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SEARCH REQUEST FORM

Access DB# 98250

NOV - 1 2002  
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(STIC)

Requester's Full Name: Zohreh Fay Examiner #: 66646 Date: 11/1/02  
Art Unit: 1614 Phone Number 308-4604 Serial Number: 091551159  
Mail Box and Bldg/Room Location: \_\_\_\_\_ Results Format Preferred (circle): PAPER DISK E-MAIL

If more than one search is submitted, please prioritize searches in order of need.

\*\*\*\*\*  
Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc., if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

Title of Invention: Beta-beta-dihydroxy morasubstituted chlorins, isobacteriochlorins and bacteriochlorins  
Inventors (please provide full names): J. H. MacAlpine, Christian Brucker, David Dolphine

Earliest Priority Filing Date: \_\_\_\_\_

\*For Sequence Searches Only\* Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.

*please search the claimed compounds, compositions and the use thereof*

*Rush Search Approved*  
*TK Page*  
*SP611615*

Jan Delaval  
Reference Librarian  
Biotechnology & Chemical Library  
CM1 1E07 - 703-308-4498  
jan.delaval@uspto.gov

STAFF USE ONLY

	Type of Search	Vendors and cost where applicable
Searcher: <u>Jan</u>	NA Sequence (#) _____	STN <input checked="" type="checkbox"/>
Searcher Phone #: <u>4498</u>	AA Sequence (#) _____	Dialog _____
Searcher Location: _____	Structure (#) <input checked="" type="checkbox"/>	Questel/Orbit _____
Date Searcher Picked Up: <u>11/3/02</u>	Bibliographic _____	Dr. Link _____
Date Completed: <u>11/3/02</u>	Litigation _____	Lexis/Nexis _____
Searcher Prep & Review Time: _____	Fulltext _____	Sequence Systems _____
Clerical Prep Time: <u>15</u>	Patent Family _____	WWW/Internet _____
Online Time: <u>50</u>	Other _____	Other (specify) _____

=> fil reg

FILE 'REGISTRY' ENTERED AT 09:48:50 ON 03 NOV 2002

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 1 NOV 2002 HIGHEST RN 469352-44-1

DICTIONARY FILE UPDATES: 1 NOV 2002 HIGHEST RN 469352-44-1

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

Please note that search-term pricing does apply when conducting SmartSELECT searches.

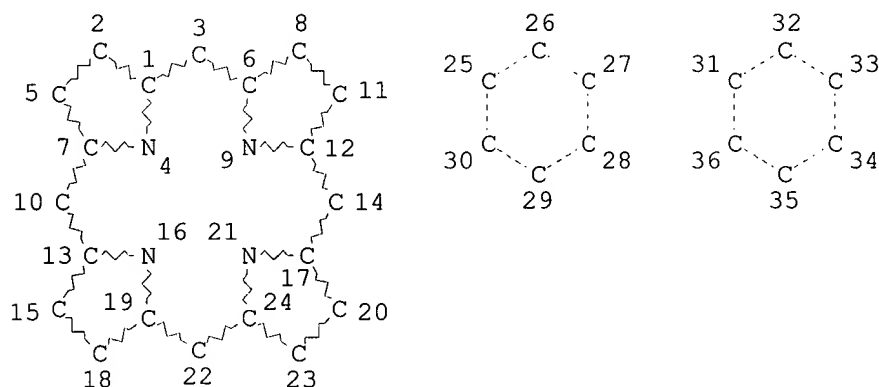
Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:

<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

=> d sta que 148

L14 STR



NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

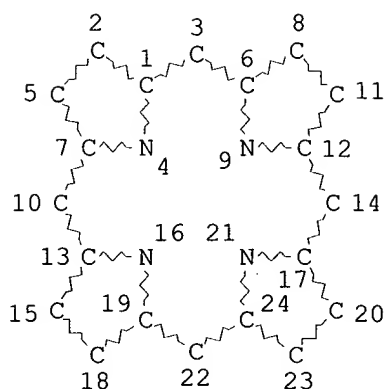
RSPEC 25 31

NUMBER OF NODES IS 36

STEREO ATTRIBUTES: NONE

L17 STR

Jan Delaval  
Reference Librarian  
Biotechnology & Chemical Library  
CM1 1E07 - 703-308-4498  
[jan.delaval@uspto.gov](mailto:jan.delaval@uspto.gov)



## NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

## GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 24

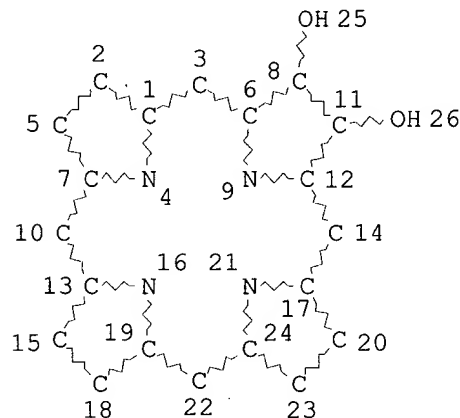
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L21 40100 SEA FILE=REGISTRY ABB=ON PLU=ON L20 AND 46.150.18/RID

L22 36698 SEA FILE=REGISTRY SUB=L21 SSS FUL L14

L23 STR



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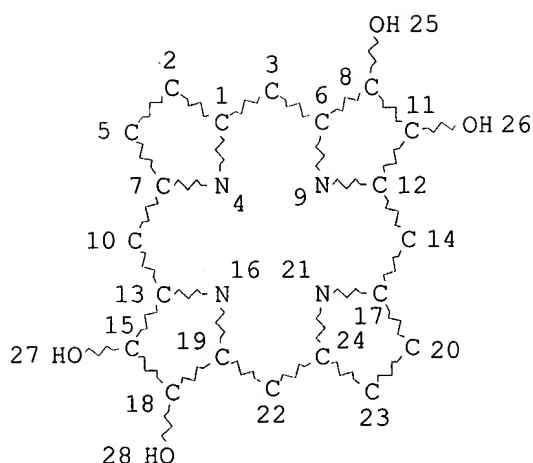
RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 26

## STEREO ATTRIBUTES: NONE

L25 102 SEA FILE=REGISTRY SUB=L22 SSS FUL L23

L27 STR



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DEFAULT ECLEVEL IS LIMITED

## GRAPH ATTRIBUTES:

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NUMBER OF NODES IS 28

## STEREO ATTRIBUTES: NONE

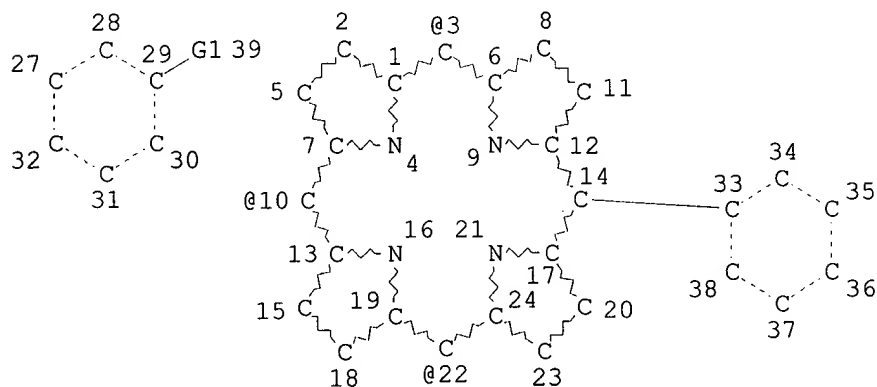
L28 30 SEA FILE=REGISTRY SUB=L25 SSS FUL L27

L29 4 SEA FILE=REGISTRY ABB=ON PLU=ON L28 AND (C44H34N4O4 OR C33H25N5O4S OR C32H26N4O4)

L30 26 SEA FILE=REGISTRY ABB=ON PLU=ON L28 NOT L29

L31 25 SEA FILE=REGISTRY ABB=ON PLU=ON L30 NOT C36H30N4O8

L34 STR



VAR G1=3/10/22

## NODE ATTRIBUTES:

CONNECT IS M3 RC AT 32

CONNECT IS M3 RC AT 36

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

## GRAPH ATTRIBUTES:

RSPEC 33 27

NUMBER OF NODES IS 37

## STEREO ATTRIBUTES: NONE

L36 75 SEA FILE=REGISTRY SUB=L25 SSS FUL L34

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L37      49 SEA FILE=REGISTRY ABB=ON  PLU=ON  L36 NOT L28
L38      1 SEA FILE=REGISTRY ABB=ON  PLU=ON  L37 AND C60H64N4O2
L39      2 SEA FILE=REGISTRY ABB=ON  PLU=ON  L37 AND (C36H28N4O6 OR
C52H40N4O10)
L40      46 SEA FILE=REGISTRY ABB=ON  PLU=ON  L37 NOT (L38 OR L39)
L41      71 SEA FILE=REGISTRY ABB=ON  PLU=ON  (L31 OR L40)
L47      3 SEA FILE=REGISTRY ABB=ON  PLU=ON  L25 AND IDS/CI
L48      74 SEA FILE=REGISTRY ABB=ON  PLU=ON  (L41 OR L47)

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SET COST OFF

FILE 'HCAPLUS' ENTERED AT 09:06:33 ON 03 NOV 2002

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      ^ E DOLPHIN D/AU
L1      484 S E3-E6
      E BRUCKNER C/AU
L2      53 S E3,E4,E11
      E MACALPINE J/AU
L3      12 S E5-E10
      E MAC ALPINE J/AU
L4      532 S L1-L3
L5      37 S L4 AND (?CHLORIN OR ?CHLORINS)
      E PORPHYRIN/CT
      E E7+ALL
L6      73912 S E4+NT
L7      189 S L4 AND L6
L8      305 S ?PORPHYR? AND L4
L9      321 S L5,L7,L8
L10     1 S L1 AND L2 AND L3
L11     531 S L4,L9 NOT L10
      SEL RN L10

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FILE 'REGISTRY' ENTERED AT 09:10:06 ON 03 NOV 2002

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L12     43 S E1-E43
L13     30 S L12 AND NR>=7
L14     STR
L15     50 S L14
L16     SCR 1868
L17     STR L14
L18     50 S L17 AND L16
L19     50 S L17
L20     71959 S L17 FUL
L21     40100 S L20 AND 46.150.18/RID
L22     36698 S L14 FUL SUB=L21
      SAV TEMP L22 FAY551/A
L23     STR L17
L24     5 S L23 SAM SUB=L22
L25     102 S L23 FUL SUB=L22
      SAV L25 FAY551A/A
L26     62 S L25 AND O>=4
L27     STR L23
L28     30 S L27 FUL SUB=L25
      SAV L28 FAY551B/A
L29     4 S L28 AND (C44H34N4O4 OR C33H25N5O4S OR C32H26N4O4)
L30     26 S L28 NOT L29
L31     25 S L30 NOT C36H30N4O8
L32     1 S L30 NOT L31
L33     STR L23
L34     STR L33
L35     2 S L34 SAM SUB=L25

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L36 75 S L34 FUL SUB=L25  
SAV L36 FAY551C/A  
L37 49 S L36 NOT L28  
L38 1 S L37 AND C60H64N4O2  
L39 2 S L37 AND (C36H28N4O6 OR C52H40N4O10)  
L40 46 S L37 NOT L38,L39  
L41 71 S L31,L40  
L42 12 S L12 AND L41  
L43 1 S L12 AND L32,L38  
L44 2 S L32,L38,L43  
L45 30 S L12 AND L20  
L46 17 S L45 NOT L41-L44  
L47 3 S L25 AND IDS/CI  
L48 74 S L41,L47  
L49 35 S L48 AND (ACETAMIDE OR ISOTHIOCYAN? OR CARBAMIC OR FE/ELS)  
L50 39 S L48 NOT L49  
SAV L48 FAY551D/A  
SAV L50 FAY551E/A

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L51 0 S L50

FILE 'HCAPLUS' ENTERED AT 09:47:18 ON 03 NOV 2002

L52 8 S L50  
L53 3 S L51 AND L1-L11  
L54 7 S L52,L53 AND (PY<=2000 OR PRY<=2000 OR AY<=2000)  
L55 2 S L44  
L56 2 S L55 AND L1-L11  
L57 8 S L52-L54  
L58 2 S L55,L56

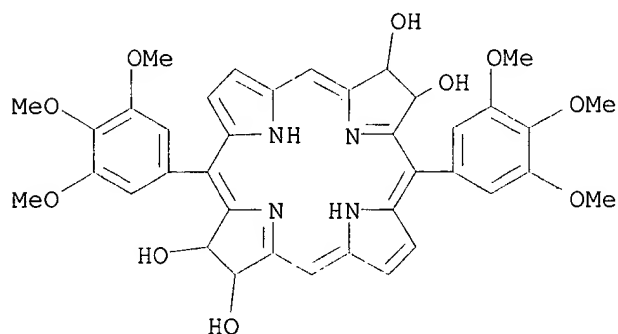
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L60 0 S L44

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L50 ANSWER 1 OF 39 REGISTRY COPYRIGHT 2002 ACS  
RN 385384-60-1 REGISTRY  
CN 21H,23H-Porphine-7,8,17,18-tetrol, 7,8,17,18-tetrahydro-5,15-bis(3,4,5-trimethoxyphenyl)- (9CI) (CA INDEX NAME)  
MF C38 H38 N4 O10  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER



Claim 16 +  
Claim 22

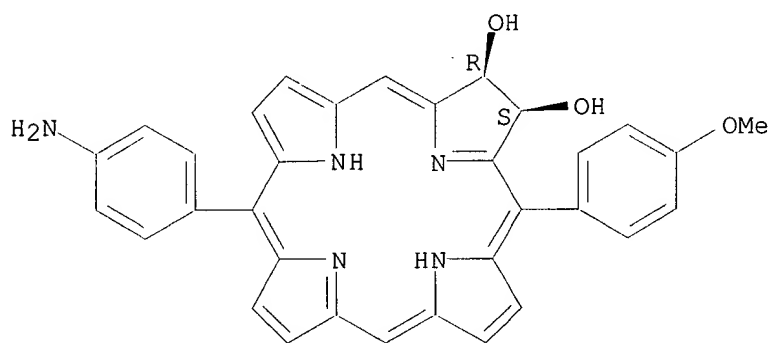
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 136:69694

L50 ANSWER 2 OF 39 REGISTRY COPYRIGHT 2002 ACS  
RN 385384-43-0 REGISTRY  
CN 21H,23H-Porphine-7,8-diol, 15-(4-aminophenyl)-7,8-dihydro-5-(4-methoxyphenyl)-, (7R,8S)-rel- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C33 H27 N5 O3  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER

Relative stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

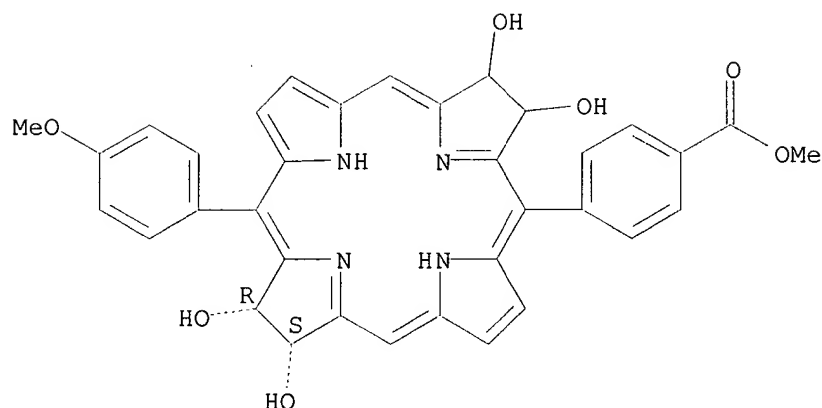
2 REFERENCES IN FILE CA (1962 TO DATE)  
2 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 136:321357

REFERENCE 2: 136:69694

L50 ANSWER 3 OF 39 REGISTRY COPYRIGHT 2002 ACS  
RN 318488-29-8 REGISTRY  
CN Benzoic acid, 4-[(17R,18S)-7,8,17,18-tetrahydro-7,8,17,18-tetrahydroxy-15-(4-methoxyphenyl)-21H,23H-porphin-5-yl]-, methyl ester, rel- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C35 H30 N4 O7  
SR CA  
LC STN Files: CA, CAPLUS, CASREACT

Relative stereochemistry.



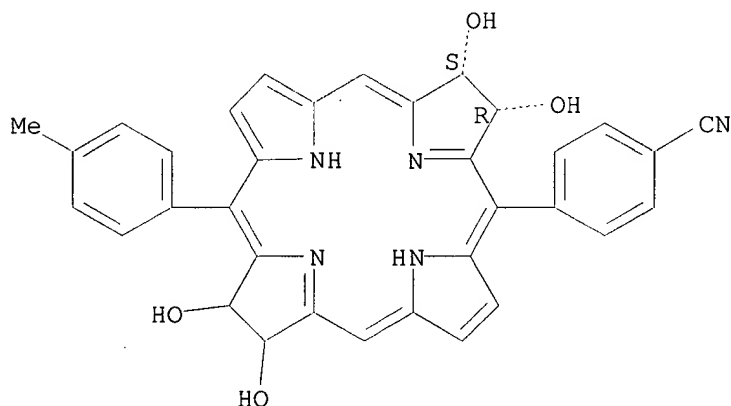
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1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 134:100684

L50 ANSWER 4 OF 39 REGISTRY COPYRIGHT 2002 ACS  
RN 318488-28-7 REGISTRY  
CN Benzonitrile, 4-[(7R,8S)-7,8,17,18-tetrahydro-7,8,17,18-tetrahydroxy-15-(4-methylphenyl)-21H,23H-porphin-5-yl]-, rel- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C34 H27 N5 O4  
SR CA  
LC STN Files: CA, CAPLUS, CASREACT

Relative stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

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1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

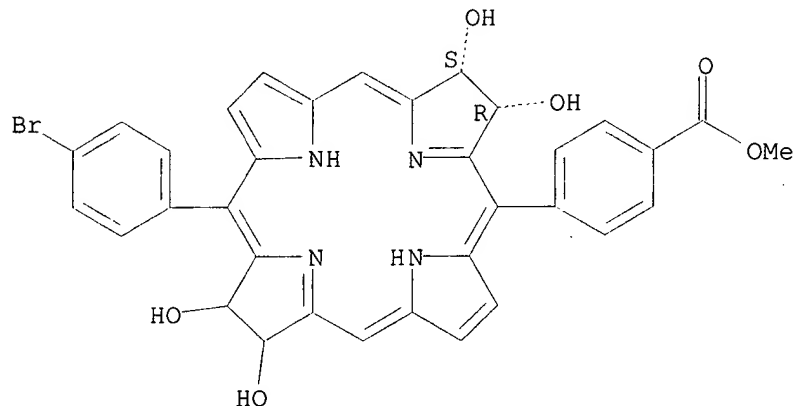
REFERENCE 1: 134:100684

L50 ANSWER 5 OF 39 REGISTRY COPYRIGHT 2002 ACS



RN 318488-27-6 REGISTRY  
CN Benzoic acid, 4-[(7R,8S)-15-(4-bromophenyl)-7,8,17,18-tetrahydro-7,8,17,18-tetrahydroxy-21H,23H-porphin-5-yl]-, methyl ester, rel- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C34 H27 Br N4 O6  
SR CA  
LC STN Files: CA, CAPLUS, CASREACT

Relative stereochemistry.



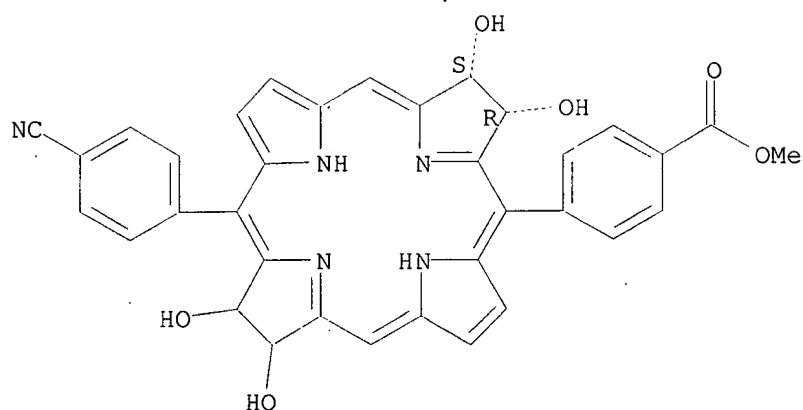
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1 REFERENCES IN FILE CA (1962 TO DATE)  
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REFERENCE 1: 134:100684

L50 ANSWER 6 OF 39 REGISTRY COPYRIGHT 2002 ACS  
RN 318488-26-5 REGISTRY  
CN Benzoic acid, 4-[(7R,8S)-15-(4-cyanophenyl)-7,8,17,18-tetrahydro-7,8,17,18-tetrahydroxy-21H,23H-porphin-5-yl]-, methyl ester, rel- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C35 H27 N5 O6  
SR CA  
LC STN Files: CA, CAPLUS, CASREACT

Relative stereochemistry.



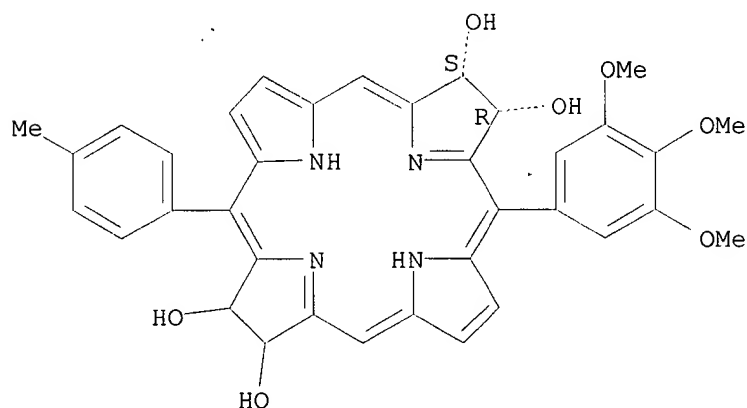
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1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 134:100684

L50 ANSWER 7 OF 39 REGISTRY COPYRIGHT 2002 ACS  
RN 318488-25-4 REGISTRY  
CN 21H,23H-Porphine-7,8,17,18-tetrol, 7,8,17,18-tetrahydro-5-(4-methylphenyl)-  
15-(3,4,5-trimethoxyphenyl)-, (17R,18S)-rel- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C36 H34 N4 O7  
SR CA  
LC STN Files: CA, CAPLUS, CASREACT

Relative stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

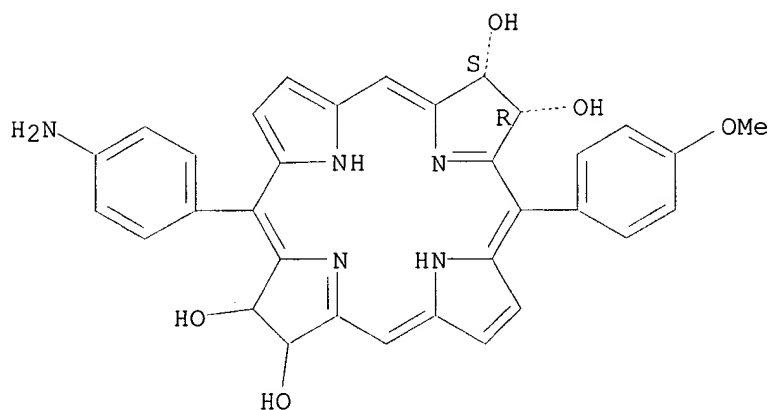
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REFERENCE 1: 134:100684

L50 ANSWER 8 OF 39 REGISTRY COPYRIGHT 2002 ACS

RN 318488-24-3 REGISTRY  
CN 21H,23H-Porphine-7,8,17,18-tetrol, 5-(4-aminophenyl)-7,8,17,18-tetrahydro-  
15-(4-methoxyphenyl)-, (17R,18S)-rel- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C33 H29 N5 O5  
SR CA  
LC STN Files: CA, CAPLUS, CASREACT

Relative stereochemistry.



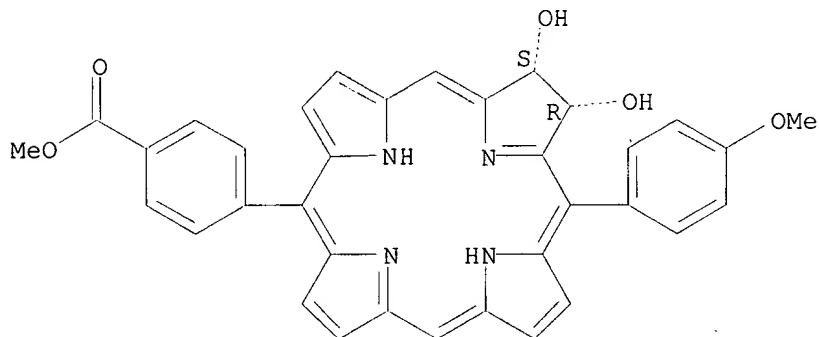
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REFERENCE 1: 134:100684

L50 ANSWER 9 OF 39 REGISTRY COPYRIGHT 2002 ACS  
RN 318488-23-2 REGISTRY  
CN Benzoic acid, 4-[(17R,18S)-17,18-dihydro-17,18-dihydroxy-15-(4-methoxyphenyl)-21H,23H-porphin-5-yl]-, methyl ester, rel- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C35 H28 N4 O5  
SR CA  
LC STN Files: CA, CAPLUS, CASREACT

Relative stereochemistry.



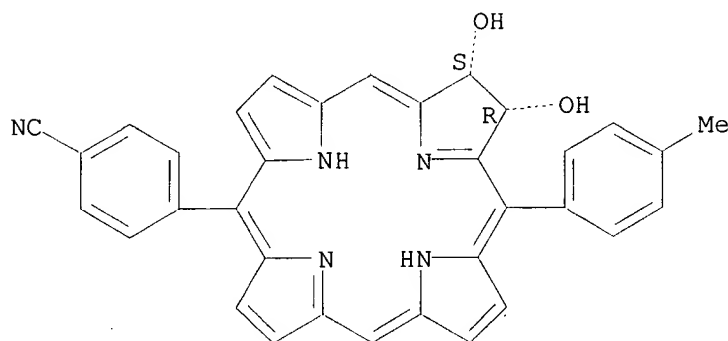
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REFERENCE 1: 134:100684

L50 ANSWER 10 OF 39 REGISTRY COPYRIGHT 2002 ACS  
RN 318488-22-1 REGISTRY  
CN Benzonitrile, 4-[(17R,18S)-17,18-dihydro-17,18-dihydroxy-15-(4-methylphenyl)-21H,23H-porphin-5-yl]-, rel- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C34 H25 N5 O2  
SR CA  
LC STN Files: CA, CAPLUS, CASREACT

Relative stereochemistry.



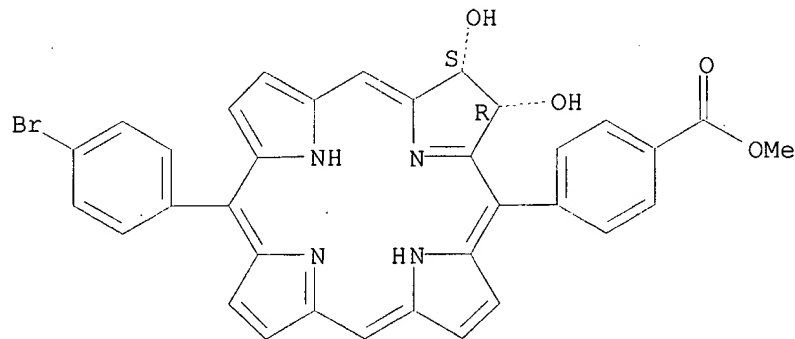
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REFERENCE 1: 134:100684

L50 ANSWER 11 OF 39 REGISTRY COPYRIGHT 2002 ACS  
RN 318488-21-0 REGISTRY  
CN Benzoic acid, 4-[(7R,8S)-15-(4-bromophenyl)-7,8-dihydro-7,8-dihydroxy-21H,23H-porphin-5-yl]-, methyl ester, rel- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C34 H25 Br N4 O4  
SR CA  
LC STN Files: CA, CAPLUS, CASREACT

Relative stereochemistry.



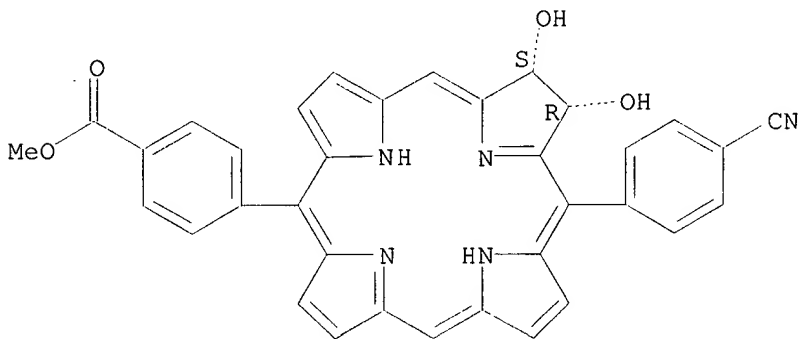
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REFERENCE 1: 134:100684

L50 ANSWER 12 OF 39 REGISTRY COPYRIGHT 2002 ACS  
RN 318488-20-9 REGISTRY  
CN Benzoic acid, 4-[(17R,18S)-15-(4-cyanophenyl)-17,18-dihydro-17,18-dihydroxy-21H,23H-porphin-5-yl]-, methyl ester, rel- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C35 H25 N5 O4  
SR CA  
LC STN Files: CA, CAPLUS, CASREACT

Relative stereochemistry.



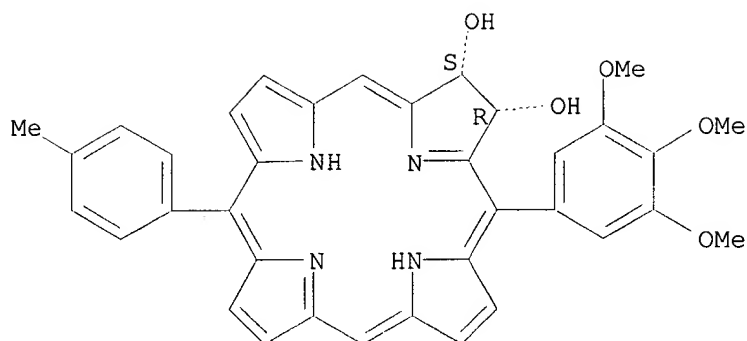
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1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 134:100684

L50 ANSWER 13 OF 39 REGISTRY COPYRIGHT 2002 ACS  
RN 318488-19-6 REGISTRY  
CN 21H,23H-Porphine-7,8-diol, 7,8-dihydro-15-(4-methylphenyl)-5-(3,4,5-trimethoxyphenyl)-, (7R,8S)-rel- (9CI) (CA INDEX NAME)  
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MF C36 H32 N4 O5  
SR CA  
LC STN Files: CA, CAPLUS, CASREACT

Relative stereochemistry.



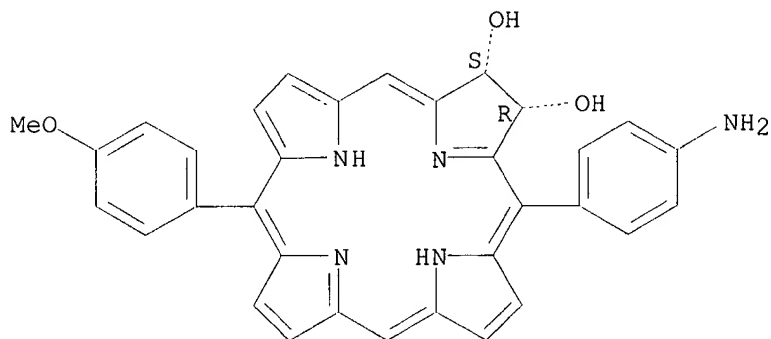
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REFERENCE 1: 134:100684

L50 ANSWER 14 OF 39 REGISTRY COPYRIGHT 2002 ACS  
RN 318488-18-5 REGISTRY  
CN 21H,23H-Porphine-7,8-diol, 5-(4-aminophenyl)-7,8-dihydro-15-(4-methoxyphenyl)-, (7R,8S)-rel- (9CI) (CA INDEX NAME)  
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MF C33 H27 N5 O3  
SR CA  
LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER

Relative stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

3 REFERENCES IN FILE CA (1962 TO DATE)  
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REFERENCE 1: 136:321357

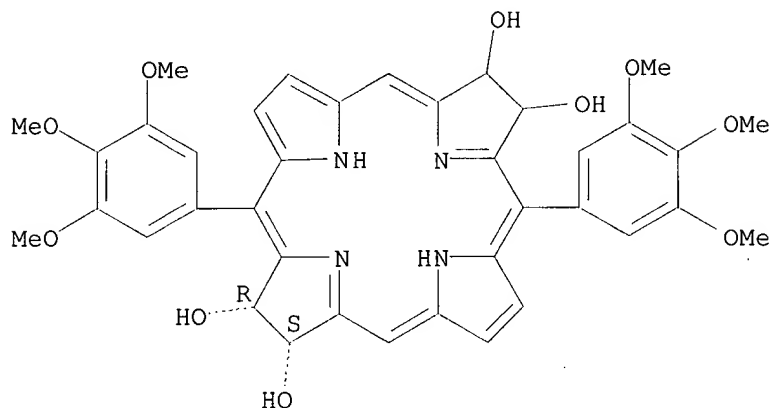
REFERENCE 2: 136:69694

REFERENCE 3: 134:100684

L50 ANSWER 15 OF 39 REGISTRY COPYRIGHT 2002 ACS  
RN 318488-12-9 REGISTRY  
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trimethoxyphenyl)-, (7R,8S)-rel- (9CI) (CA INDEX NAME)  
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 MF C38.H38 N4 O10  
 SR CA  
 LC STN Files: CA, CAPLUS, CASREACT

Relative stereochemistry.



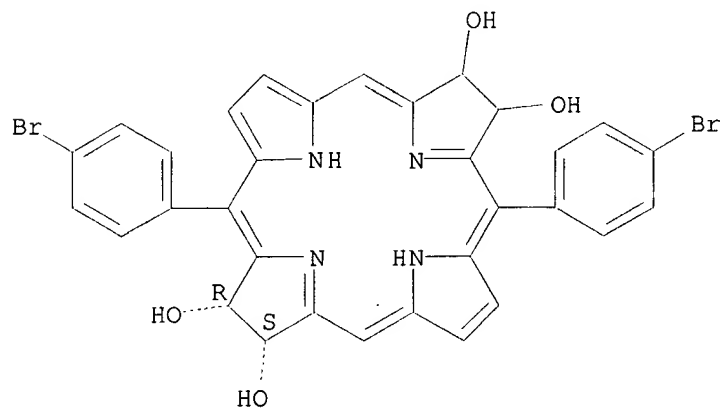
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 1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 134:100684

L50 ANSWER 16 OF 39 REGISTRY COPYRIGHT 2002 ACS  
 RN 318488-10-7 REGISTRY  
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 FS STEREOSEARCH  
 MF C32 H24 Br2 N4 O4  
 SR CA  
 LC STN Files: CA, CAPLUS, CASREACT

Relative stereochemistry.



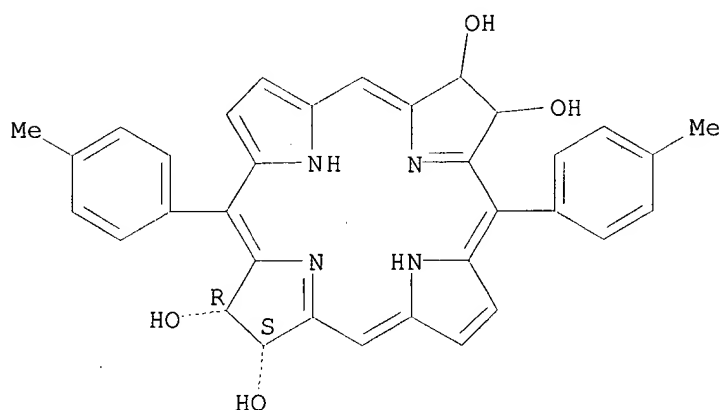
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 134:100684

L50 ANSWER 17 OF 39 REGISTRY COPYRIGHT 2002 ACS  
RN 318488-08-3 REGISTRY  
CN 21H,23H-Porphine-7,8,17,18-tetrol, 7,8,17,18-tetrahydro-5,15-bis(4-methylphenyl)-, (7R,8S)-rel- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C34 H30 N4 O4  
SR CA  
LC STN Files: CA, CAPLUS, CASREACT

Relative stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

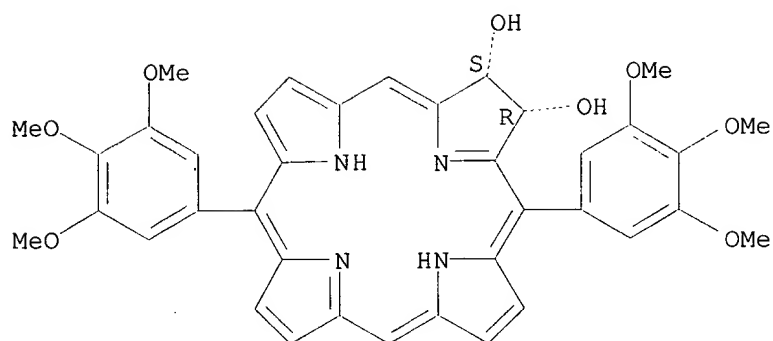
1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 134:100684

L50 ANSWER 18 OF 39 REGISTRY COPYRIGHT 2002 ACS  
RN 318488-06-1 REGISTRY  
CN 21H,23H-Porphine-7,8-diol, 7,8-dihydro-5,15-bis(3,4,5-trimethoxyphenyl)-, (7R,8S)-rel- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C38 H36 N4 O8  
SR CA  
LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER

Relative stereochemistry.





\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

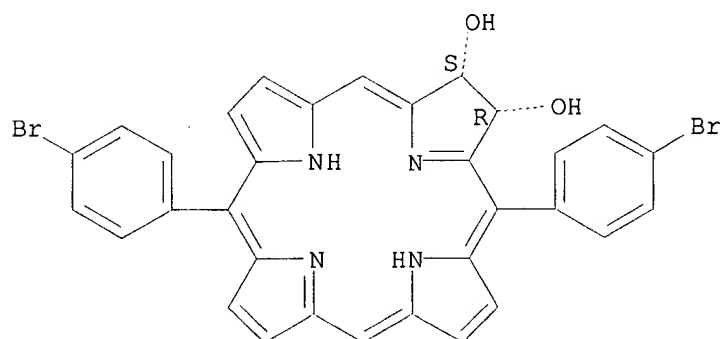
2 REFERENCES IN FILE CA (1962 TO DATE)  
2 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 136:69694

REFERENCE 2: 134:100684

L50 ANSWER 19 OF 39 REGISTRY COPYRIGHT 2002 ACS  
RN 318488-04-9 REGISTRY  
CN 21H,23H-Porphine-7,8-diol, 5,15-bis(4-bromophenyl)-7,8-dihydro-,  
(7R,8S)-rel- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C32 H22 Br2 N4 O2  
SR CA  
LC STN Files: CA, CAPLUS, CASREACT

Relative stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

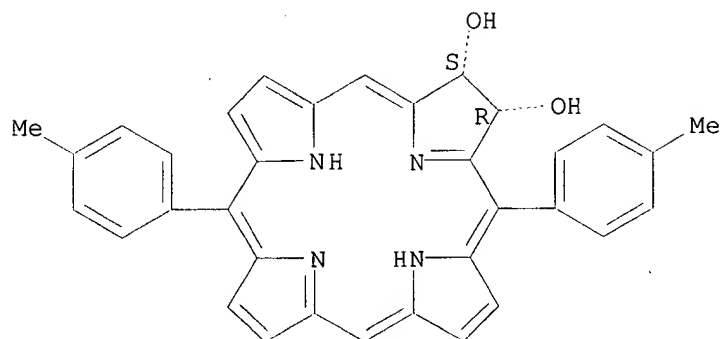
1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 134:100684

L50 ANSWER 20 OF 39 REGISTRY COPYRIGHT 2002 ACS  
RN 318488-03-8 REGISTRY  
CN 21H,23H-Porphine-7,8-diol, 7,8-dihydro-5,15-bis(4-methylphenyl)-,  
(7R,8S)-rel- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH

MF C34 H28 N4 O2  
 SR CA  
 LC STN Files: CA, CAPLUS, CASREACT

Relative stereochemistry.

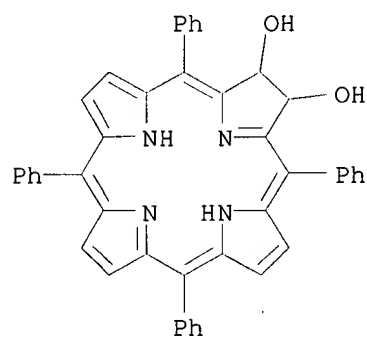


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1962 TO DATE)  
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REFERENCE 1: 134:100684

L50 ANSWER 21 OF 39 REGISTRY COPYRIGHT 2002 ACS  
 RN 301530-03-0 REGISTRY  
 CN 21H,23H-Porphine-7,8-diol, 7,8-dihydro-5(or 15)-(4-nitrophenyl)-  
 10,15,20(or 5,10,20)-triphenyl-, (7R,8R)-rel- (9CI) (CA INDEX NAME)  
 MF C44 H31 N5 O4  
 CI IDS  
 SR CA  
 LC STN Files: CA, CAPLUS, TOXCENTER



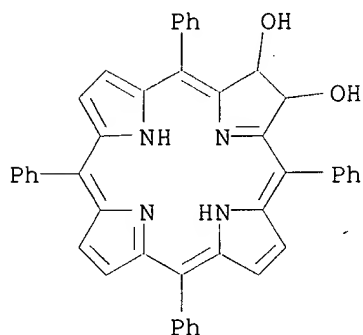
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REFERENCE 1: 133:296322

L50 ANSWER 22 OF 39 REGISTRY COPYRIGHT 2002 ACS  
 RN 301530-02-9 REGISTRY

CN 21H,23H-Porphine-7,8-diol, 7,8-dihydro-5(or 15)-(4-hydroxyphenyl)-  
10,15,20(or 5,10,20)-triphenyl-, (7R,8R)-rel- (9CI) (CA INDEX NAME)  
MF C44 H32 N4 O3  
CI IDS  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER

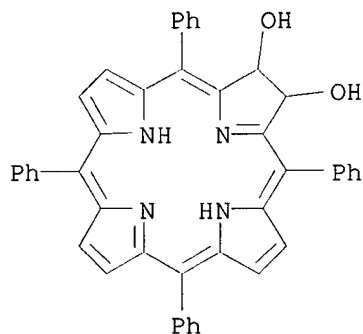


D1-OH

1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 133:296322

L50 ANSWER 23 OF 39 REGISTRY COPYRIGHT 2002 ACS  
RN 301530-01-8 REGISTRY  
CN 21H,23H-Porphine-7,8-diol, 5(or 15)-(4-bromophenyl)-7,8-dihydro-  
10,15,20(or 5,10,20)-triphenyl-, (7R,8R)-rel- (9CI) (CA INDEX NAME)  
MF C44 H31 Br N4 O2  
CI IDS  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER



D1-Br

1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

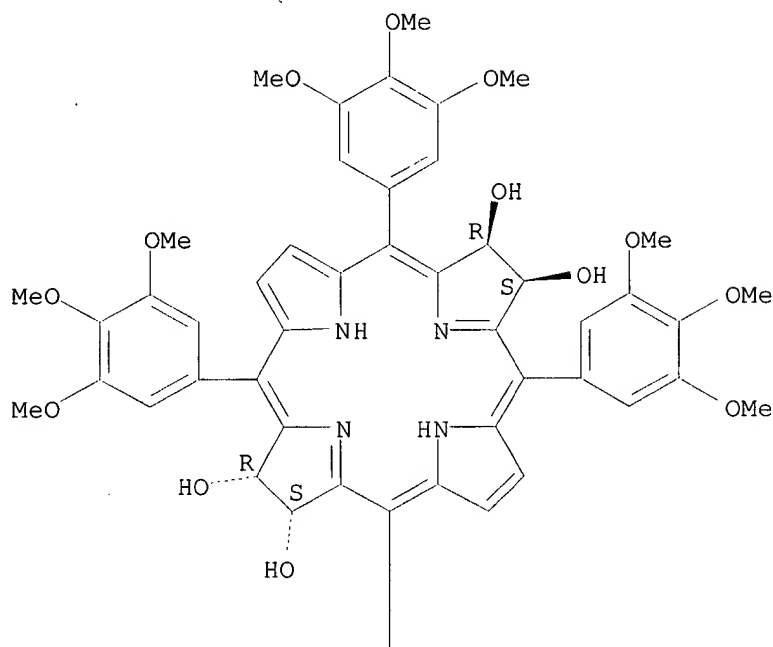
REFERENCE 1: 133:296322

L50 ANSWER 24 OF 39 REGISTRY COPYRIGHT 2002 ACS

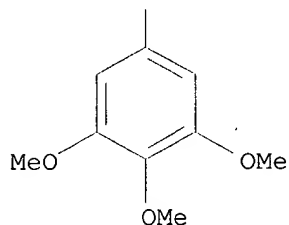
RN 301337-23-5 REGISTRY  
 CN 21H,23H-Porphine-7,8,17,18-tetrol, 7,8,17,18-tetrahydro-5,10,15,20-tetrakis(3,4,5-trimethoxyphenyl)-, (7R,8S,17S,18R)-rel- (9CI) (CA INDEX NAME)  
 FS STEREOSEARCH  
 MF C56 H58 N4 O16  
 SR CA  
 LC STN Files: CA, CAPLUS, TOXCENTER

Relative stereochemistry.

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1 REFERENCES IN FILE CA (1962 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

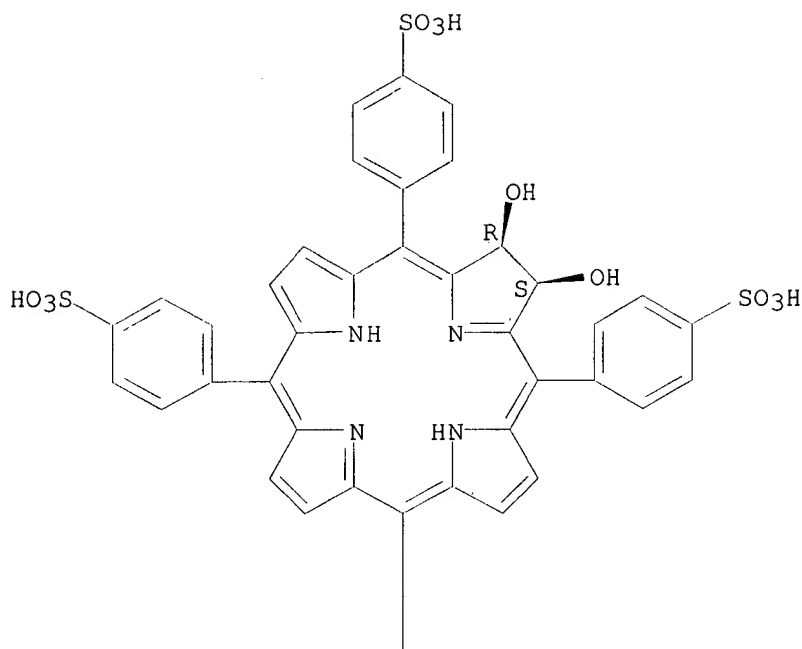
REFERENCE 1: 133:296322

L50 ANSWER 25 OF 39 REGISTRY COPYRIGHT 2002 ACS  
 RN 301337-16-6 REGISTRY  
 CN Benzenesulfonic acid, 4,4',4'',4'''-[(7R,8S)-7,8-dihydro-7,8-dihydroxy-21H,23H-porphine-5,10,15,20-tetrayl]tetrakis-, rel- (9CI) (CA INDEX NAME)  
 FS STEREOSEARCH  
 MF C44 H32 N4 O14 S4

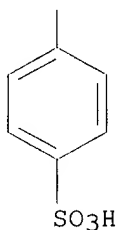
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER

Relative stereochemistry.

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\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

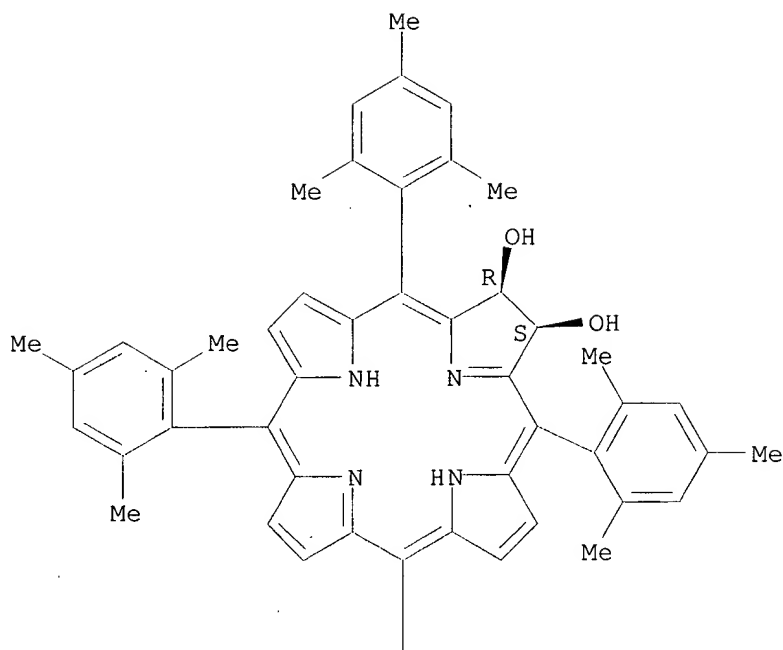
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REFERENCE 1: 133:296322

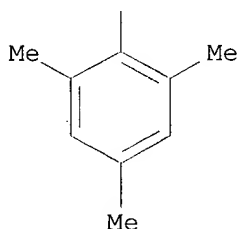
L50 ANSWER 26 OF 39 REGISTRY COPYRIGHT 2002 ACS  
RN 301337-13-3 REGISTRY  
CN 21H,23H-Porphine-7,8-diol, 7,8-dihydro-5,10,15,20-tetrakis(2,4,6-trimethylphenyl)-, (7R,8S)-rel- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C56 H56 N4 O2  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER

Relative stereochemistry.

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\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

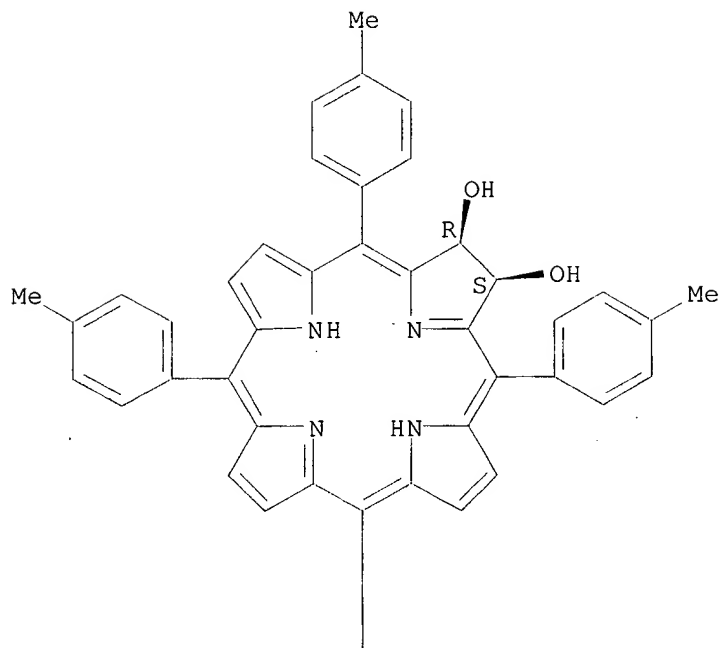
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REFERENCE 1: 133:296322

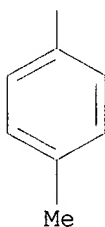
L50 ANSWER 27 OF 39 REGISTRY COPYRIGHT 2002 ACS  
 RN 301337-10-0 REGISTRY  
 CN 21H,23H-Porphine-7,8-diol, 7,8-dihydro-5,10,15,20-tetrakis(4-methylphenyl)-  
 , (7R,8S)-rel- (9CI) (CA INDEX NAME)  
 FS STEREOSEARCH  
 MF C48 H40 N4 O2  
 SR CA  
 LC STN Files: CA, CAPLUS, TOXCENTER

Relative stereochemistry.

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\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

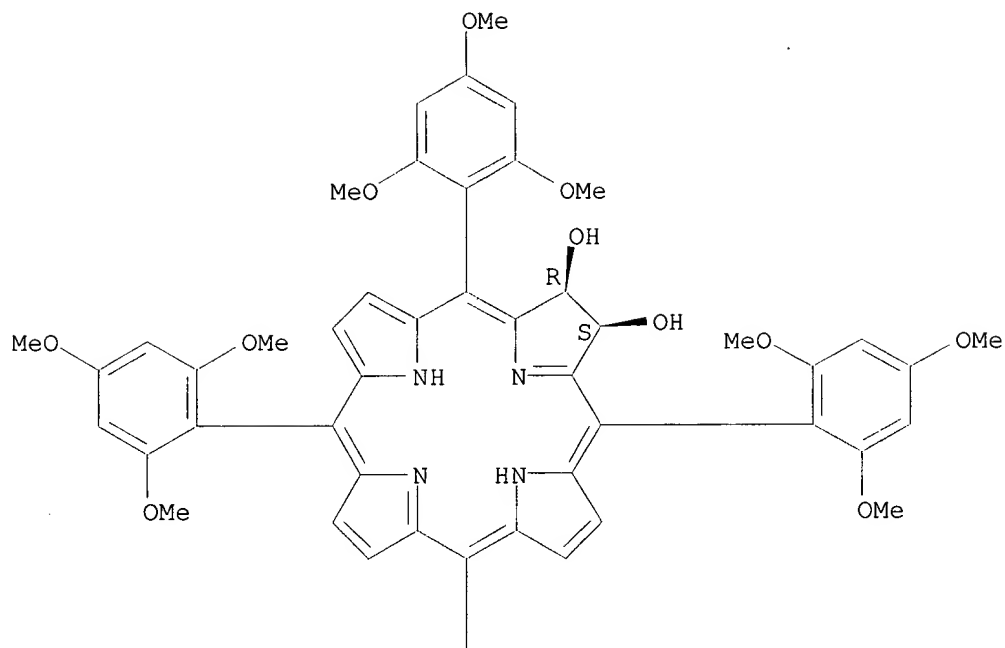
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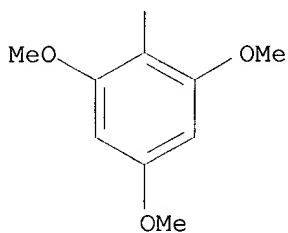
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L50  ANSWER 28 OF 39  REGISTRY  COPYRIGHT 2002 ACS
RN   301337-07-5  REGISTRY
CN   21H,23H-Porphine-7,8-diol, 7,8-dihydro-5,10,15,20-tetrakis(2,4,6-
trimethoxyphenyl)-, (7R,8S)-rel- (9CI)  (CA INDEX NAME)
FS.  STEREOSEARCH
MF   C56 H56 N4 O14
SR   CA
LC   STN Files:    CA, CAPLUS, TOXCENTER
```

Relative stereochemistry.

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\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

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1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

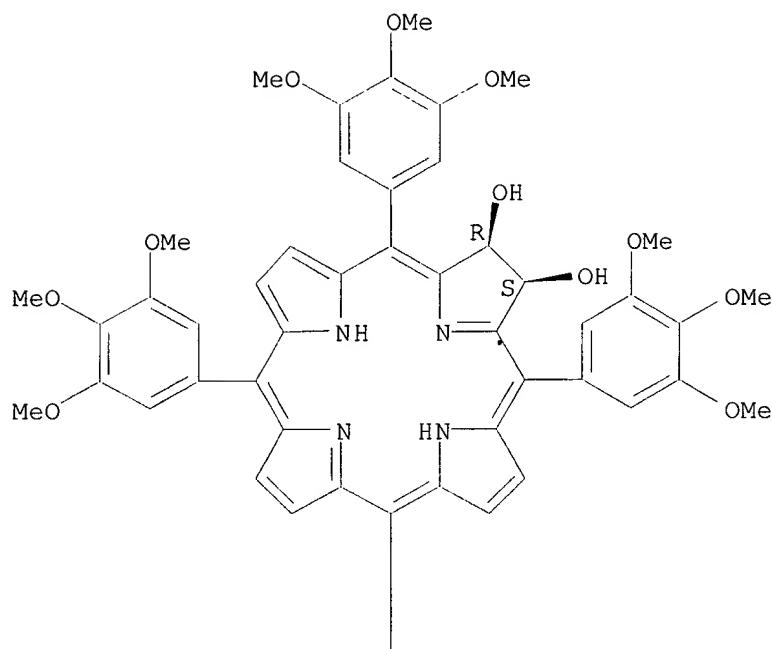
REFERENCE 1: 133:296322

L50 ANSWER 29 OF 39 REGISTRY COPYRIGHT 2002 ACS  
RN 301337-03-1 REGISTRY  
CN 21H,23H-Porphine-7,8-diol, 7,8-dihydro-5,10,15,20-tetrakis(3,4,5-trimethoxyphenyl)-, (7R,8S)-rel- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C56 H56 N4 O14  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER

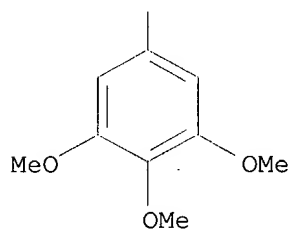
Relative stereochemistry.



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\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

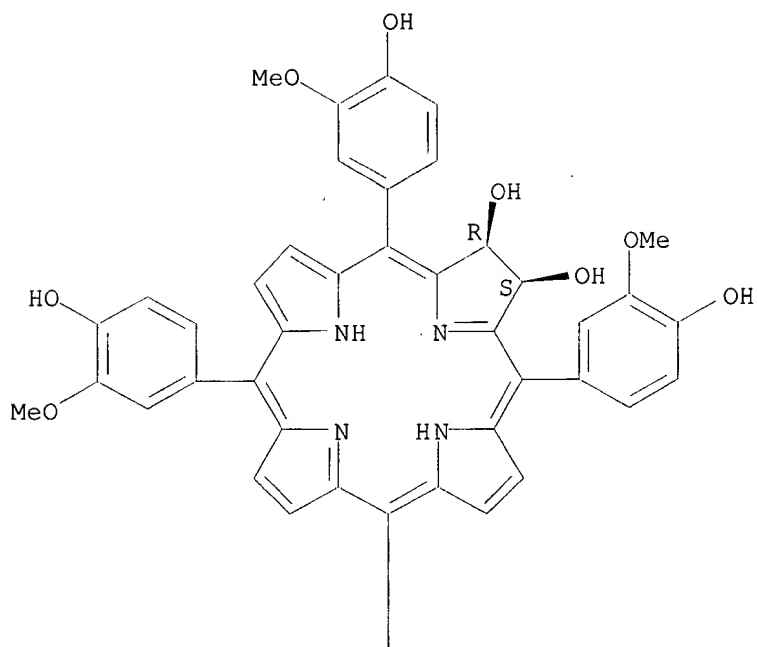
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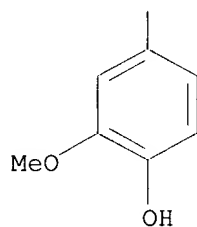
L50 ANSWER 30 OF 39 REGISTRY COPYRIGHT 2002 ACS  
RN 301337-00-8 REGISTRY  
CN 21H,23H-Porphine-7,8-diol, 7,8-dihydro-5,10,15,20-tetrakis(4-hydroxy-3-methoxyphenyl)-, (7R,8S)-rel- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C48 H40 N4 O10  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER

Relative stereochemistry.

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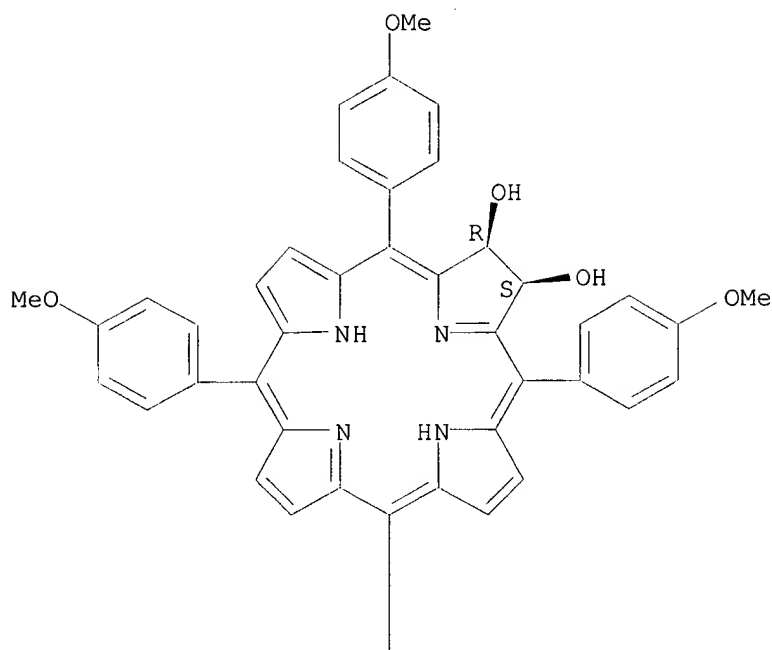
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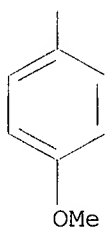
L50 ANSWER 31 OF 39 REGISTRY COPYRIGHT 2002 ACS  
 RN 301336-91-4 REGISTRY  
 CN 21H,23H-Porphine-7,8-diol, 7,8-dihydro-5,10,15,20-tetrakis(4-methoxyphenyl)-, (7R,8S)-rel- (9CI) (CA INDEX NAME)  
 FS STEREOSEARCH  
 MF C48 H40 N4 O6  
 SR CA  
 LC STN Files: CA, CAPLUS, TOXCENTER

Relative stereochemistry.

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\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

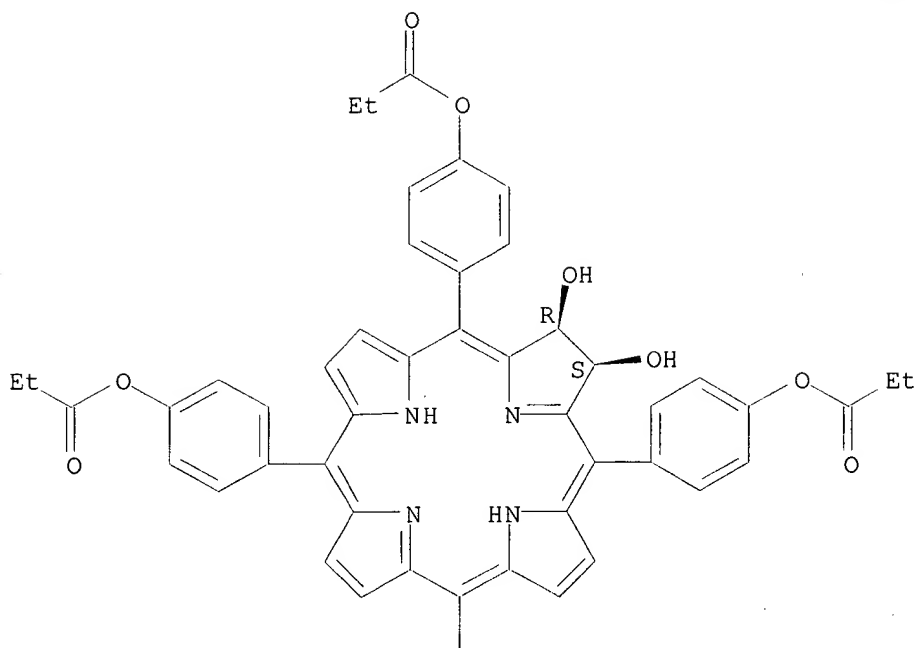
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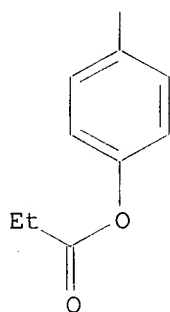
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L50  ANSWER 32 OF 39  REGISTRY  COPYRIGHT 2002 ACS
RN   301336-88-9  REGISTRY
CN   21H,23H-Porphine-7,8-diol, 7,8-dihydro-5,10,15,20-tetrakis[4-(1-oxopropoxy)phenyl]-, (7R,8S)-rel- (9CI)  (CA INDEX NAME)
FS   STEREOSEARCH
MF   C56 H48 N4 O10
SR   CA
LC   STN Files:    CA, CAPLUS, TOXCENTER
```

Relative stereochemistry.

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\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

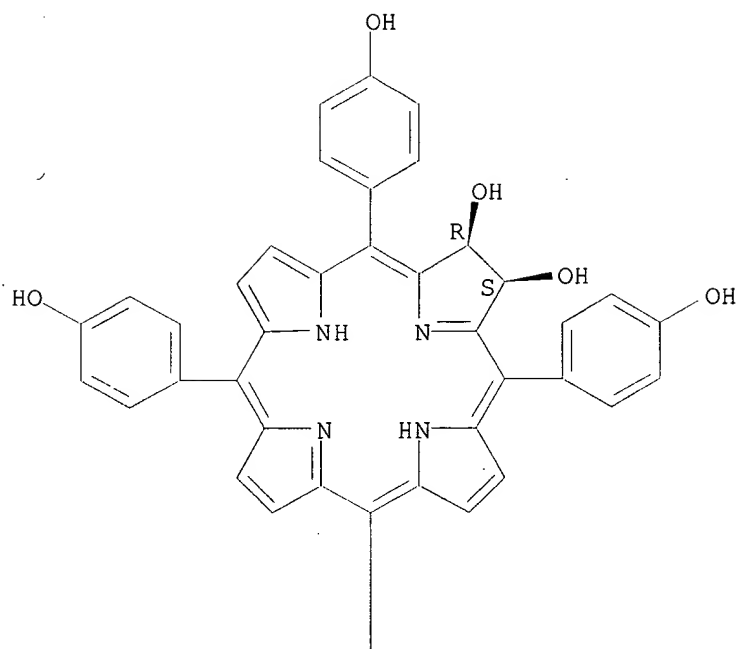
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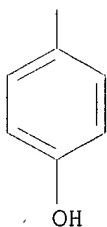
L50 ANSWER 33 OF 39 REGISTRY COPYRIGHT 2002 ACS  
RN 301336-78-7 REGISTRY  
CN 21H,23H-Porphine-7,8-diol, 7,8-dihydro-5,10,15,20-tetrakis(4-hydroxyphenyl)-, (7R,8S)-rel- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C44 H32 N4 O6  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER

Relative stereochemistry.

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\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

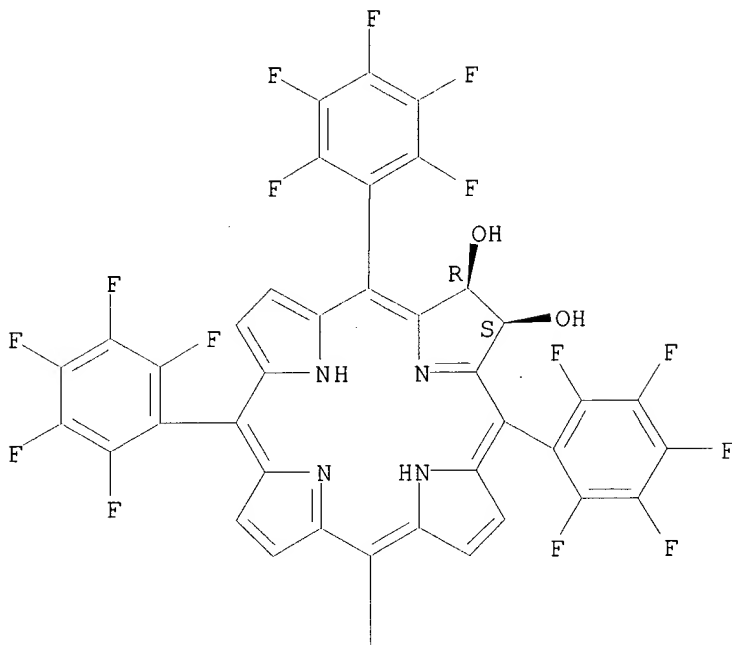
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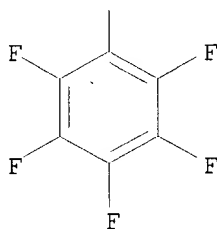
L50 ANSWER 34 OF 39 REGISTRY COPYRIGHT 2002 ACS  
RN 301336-74-3 REGISTRY  
CN 21H,23H-Porphine-7,8-diol, 7,8-dihydro-5,10,15,20-  
tetrakis(pentafluorophenyl)-, (7R,8S)-rel- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C44 H12 F20 N4 O2  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER

Relative stereochemistry.

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\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

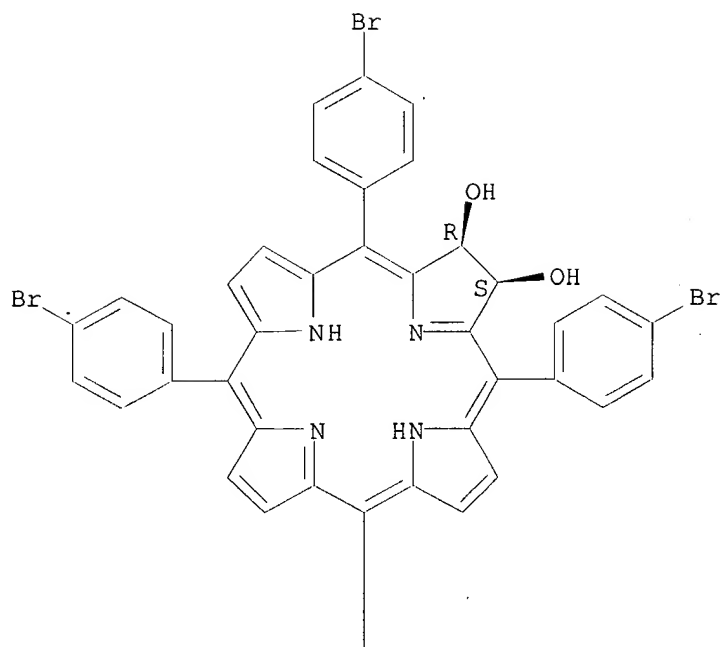
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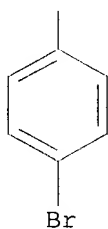
L50 ANSWER 35 OF 39 REGISTRY COPYRIGHT 2002 ACS  
RN 301336-61-8 REGISTRY  
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, (7R,8S)-rel- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C44 H28 Br4 N4 O2  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER

Relative stereochemistry.

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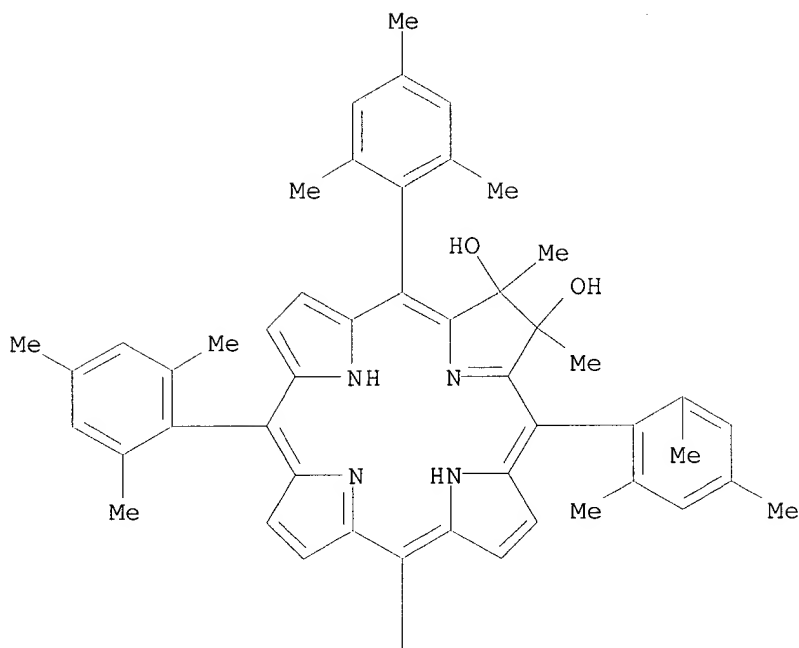
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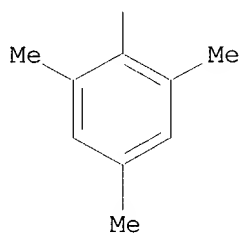
REFERENCE 1: 133:296322

L50 ANSWER 36 OF 39 REGISTRY COPYRIGHT 2002 ACS  
RN 167936-43-8 REGISTRY  
CN 21H,23H-Porphine-7,8-diol, 7,8-dihydro-7,8-dimethyl-5,10,15,20-tetrakis(2,4,6-trimethylphenyl)-, radical ion(1+), (7R,8R)-rel- (9CI) (CA INDEX NAME)  
MF C58 H60 N4 O2  
SR CA  
LC STN Files: CA, CAPLUS

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\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

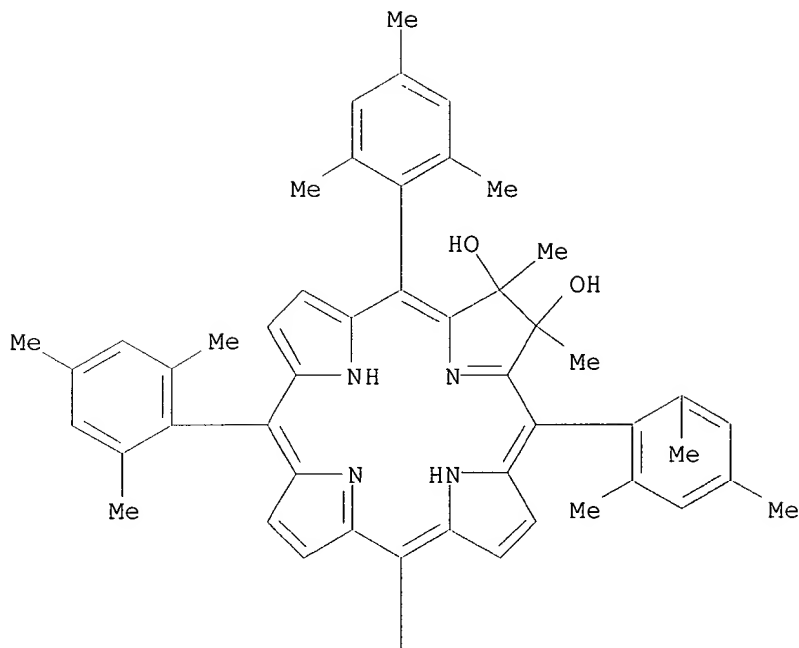
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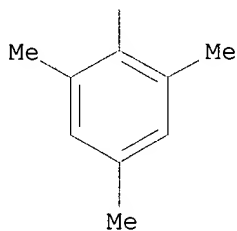
L50 ANSWER 37 OF 39 REGISTRY COPYRIGHT 2002 ACS  
RN 167774-51-8 REGISTRY  
CN 21H,23H-Porphine-7,8-diol, 7,8-dihydro-7,8-dimethyl-5,10,15,20-  
tetakis(2,4,6-trimethylphenyl)-, (7R,8R)-rel- (9CI) (CA INDEX NAME)  
MF C58 H60 N4 O2  
SR CA  
LC STN Files: CA, CAPLUS



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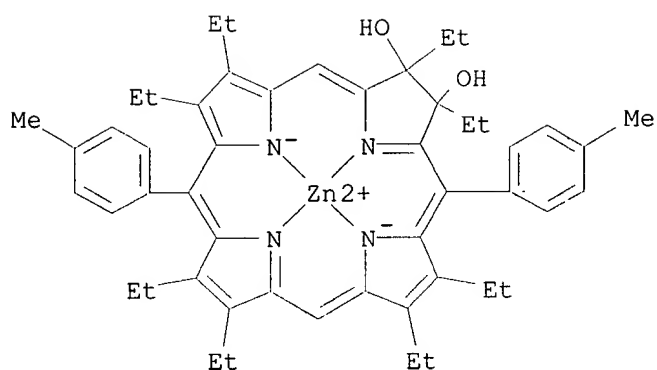


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

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REFERENCE 1: 123:216794

L50 ANSWER 38 OF 39 REGISTRY COPYRIGHT 2002 ACS  
 RN 155737-01-2 REGISTRY  
 CN Zinc, [rel-(7R,8S)-2,3,7,8,12,13,17,18-octaethyl-7,8-dihydro-5,15-bis(4-methylphenyl)-21H,23H-porphine-7,8-diolato(2-)-.kappa.N21,.kappa.N22,.kappa.N23,.kappa.N24]-, (SP-4-2)- (9CI) (CA INDEX NAME)  
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 CI CCS  
 SR CA  
 LC STN Files: CA, CAPLUS

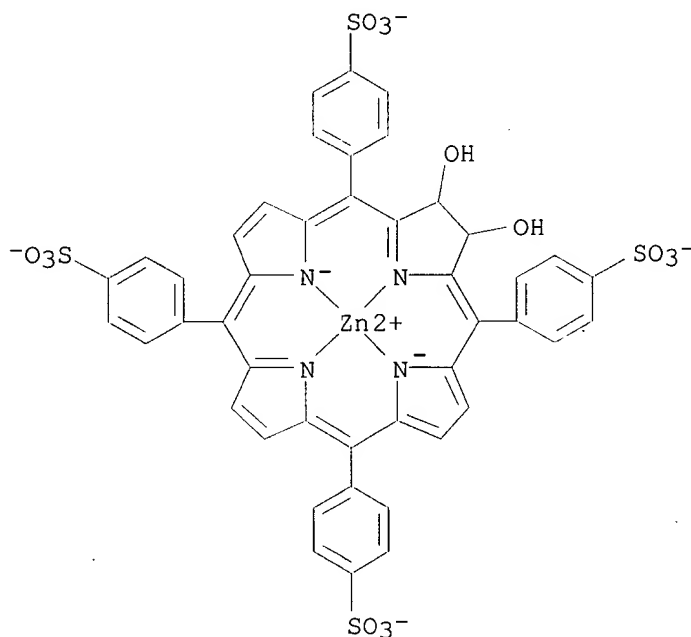


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1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 121:8966

L50 ANSWER 39 OF 39 REGISTRY COPYRIGHT 2002 ACS  
RN 133551-73-2 REGISTRY  
CN Zincate(4-), [[4,4',4'',4'''-(7,8-dihydro-7,8-dihydroxy-21H,23H-porphine-5,10,15,20-tetrayl-.kappa.N21,.kappa.N22,.kappa.N23,.kappa.N24)tetrakis(benzenesulfonato)](6-)]-, tetrahydrogen, (SP-4-1)-(9CI) (CA INDEX NAME)  
MF C44 H26 N4 O14 S4 Zn . 4 H  
CI CCS  
SR CA  
LC STN Files: CA, CAPLUS

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4 H<sup>+</sup>

2 REFERENCES IN FILE CA (1962 TO DATE)  
2 REFERENCES IN FILE CAPLUS (1962 TO DATE)

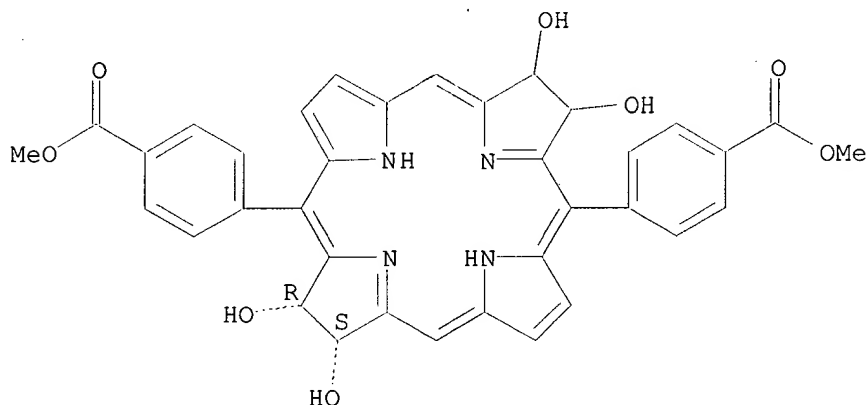
REFERENCE 1: 115:18425

REFERENCE 2: 114:217823

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L44 ANSWER 1 OF 2 REGISTRY COPYRIGHT 2002 ACS  
RN 318488-11-8 REGISTRY  
CN Benzoic acid, 4,4'-[(7R,8S)-7,8,17,18-tetrahydro-7,8,17,18-tetrahydroxy-21H,23H-porphine-5,15-diyl]bis-, dimethyl ester, rel- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C36 H30 N4 O8  
SR CA  
LC STN Files: CA, CAPLUS, CASREACT

Relative stereochemistry.



FYI - porphyrin-  
excluded as per  
page 4

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

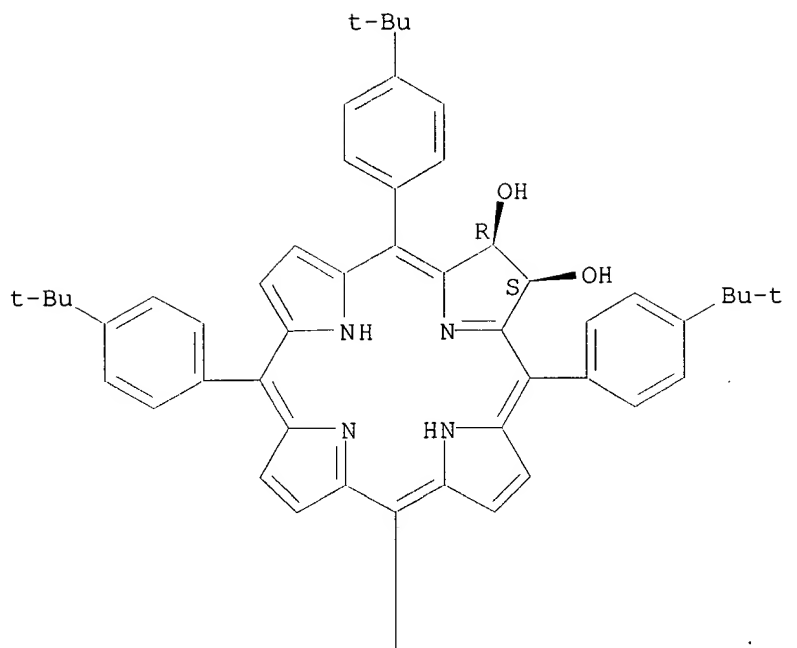
1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 134:100684

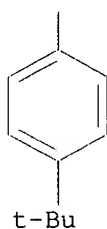
L44 ANSWER 2 OF 2 REGISTRY COPYRIGHT 2002 ACS  
RN 301337-19-9 REGISTRY  
CN 21H,23H-Porphine-7,8-diol, 5,10,15,20-tetrakis[4-(1,1-dimethylethyl)phenyl]-7,8-dihydro-, (7R,8S)-rel- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C60 H64 N4 O2  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER

Relative stereochemistry.

PAGE 1-A



PAGE 2-A



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 133:296322

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FILE LAST UPDATED: 1 Nov 2002 (20021101/ED)

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=> d all tot 158 hitstr

L58 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2002 ACS  
AN 2000:831421 HCAPLUS  
DN 134:100684  
TI Functionalized diphenylchlorins and bacteriochlorins: their synthesis and bioconjugation for targeted photodynamic therapy and tumor cell imaging  
AU Sutton, Jonathan M.; Fernandez, Nelson; Boyle, Ross W.  
CS Department of Biological Sciences, University of Essex, Colchester, CO4 3SQ, UK  
SO Journal of Porphyrins and Phthalocyanines (2000), 4(7), 655-658  
CODEN: JPPHFZ; ISSN: 1088-4246  
PB John Wiley & Sons Ltd.  
DT Journal  
LA English  
CC 26-7 (Biomolecules and Their Synthetic Analogs)  
Section cross-reference(s): 9, 22  
OS CASREACT 134:100684  
AB A range of 5,15-diphenylporphyrins with sym. and unsym. substitution patterns were subjected to osmium tetroxide-mediated dihydroxylations. The resulting chlorins and bacteriochlorins present an important group of compds. for studying structure-activity relationships of photodynamic sensitizers. The regioselectivity of the dihydroxylation of various 5,15-diphenylporphyrins with unsym. substitution patterns was also examd. Both diphenylchlorin diol (DPC) and diphenylbacteriochlorin tetrol (DPBC) examples were converted into reactive isothiocyanates and conjugated with bovine serum albumin (BSA).  
ST porphyrin diphenyl dihydroxylation regioselective; chlorin diphenyl dihydroxy tetrahydroxy prepn; diphenylchlorin bacteriochlorin isothiocyanate conjugate BSA  
IT **Porphyrins**  
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (chlorins, di-Ph; synthesis and bioconjugation of functionalized diphenylchlorins and bacteriochlorins for targeted photodynamic therapy and tumor cell imaging)  
IT Albumins, biological studies  
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process) (conjugates; synthesis and bioconjugation of functionalized diphenylchlorins and bacteriochlorins for targeted photodynamic therapy and tumor cell imaging)  
IT Dihydroxylation  
(stereoselective; synthesis and bioconjugation of functionalized diphenylchlorins and bacteriochlorins for targeted photodynamic therapy and tumor cell imaging)  
IT Fluorescence  
UV and visible spectra

(synthesis and bioconjugation of functionalized diphenylchlorins and bacteriochlorins for targeted photodynamic therapy and tumor cell imaging)

IT 318488-18-5P 318488-24-3P  
 RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (synthesis and bioconjugation of functionalized diphenylchlorins and bacteriochlorins for targeted photodynamic therapy and tumor cell imaging)

IT 318488-06-1P 318488-12-9P 318488-23-2P 318488-29-8P 318488-30-1DP, conjugate with BSA 318488-31-2DP, conjugate with BSA  
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
 (synthesis and bioconjugation of functionalized diphenylchlorins and bacteriochlorins for targeted photodynamic therapy and tumor cell imaging)

IT 22112-89-6, 5,15-Diphenylporphyrin 128374-05-0 253666-33-0 268737-71-9 318488-01-6 318488-02-7 318488-13-0 318488-14-1 318488-15-2 318488-16-3 318488-17-4  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (synthesis and bioconjugation of functionalized diphenylchlorins and bacteriochlorins for targeted photodynamic therapy and tumor cell imaging)

IT 165336-21-0P 318488-03-8P 318488-04-9P 318488-05-0P 318488-07-2P 318488-08-3P 318488-10-7P **318488-11-8P** 318488-19-6P 318488-20-9P 318488-21-0P 318488-22-1P 318488-25-4P 318488-26-5P 318488-27-6P 318488-28-7P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (synthesis and bioconjugation of functionalized diphenylchlorins and bacteriochlorins for targeted photodynamic therapy and tumor cell imaging)

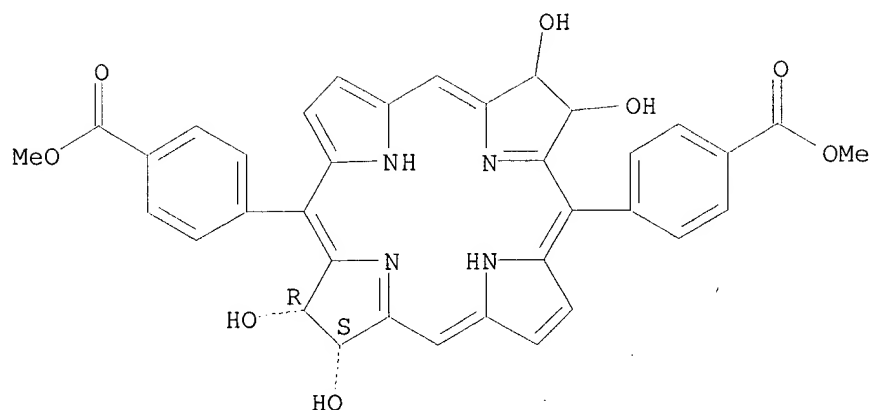
RE.CNT 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD  
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 (18) Sternberg, E; Tetrahedron 1998, V54, P4151 HCAPLUS

IT **318488-11-8P**  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (synthesis and bioconjugation of functionalized diphenylchlorins and bacteriochlorins for targeted photodynamic therapy and tumor cell imaging)

RN 318488-11-8 HCAPLUS

CN Benzoic acid, 4,4'-[(7R,8S)-7,8,17,18-tetrahydro-7,8,17,18-tetrahydroxy-21H,23H-porphine-5,15-diyl]bis-, dimethyl ester, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L58 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2002 ACS

AN 2000:742097 HCAPLUS

DN 133:296322

TI Synthesis of .beta.,.beta.,-dihydroxymeso-substituted **chlorins**, **isobacteriochlorins**, and **bacteriochlorins** with improved photosensitizer activity

IN Macalpine, Jill; Dolphin, David; Bruckner, Christian

PA University of British Columbia, Can.

SO PCT Int. Appl., 53 pp.

CODEN: PIXXD2

DT Patent

LA English

IC ICM C07D487-22

ICS A61K031-409; A61K049-00; A61P035-00; C07D487-22; C07D257-00;

C07D209-00; C07D209-00; C07D209-00; C07D209-00

CC 26-7 (Biomolecules and Their Synthetic Analogs)

Section cross-reference(s): 1, 8

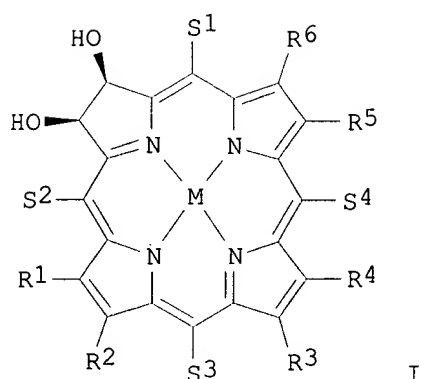
FAN.CNT 2

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000061584	A1	20001019	WO 2000-CA435	20000414
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				

PRAI US 1999-129324P P 19990414

OS MARPAT 133:296322

GI



- AB Synthesis of .beta.,.beta.,-dihydroxymeso-substituted **chlorins** (I) [M = 2H, Ni(II), Cu(II), Zn, Sn, Ge, Si, Ga, Al, Mn(III), Gd(III), In, Tc; R1-R6 = independently H, alkyl, alkylcarboxylic acid or ester, =O, OH, NO<sub>2</sub>, NH<sub>2</sub>; taken together with another ring, ring substituent or meso substituent = fused 5- or 6-membered ring; S1-S4 independently = H, (un)substituted alkyl, (un)substituted aryl, (un)substituted cycloalkyl, may be same or different], **bacteriochlorins**, and **isobacteriochlorins** with improved photosensitizer activity is described. Thus, I (S1-S4 = Ph, M = 2H, R1-R6 = H) (II) is prepd. by treatment of **tetraphenylporphyrin** with osmium tetroxide. II shows an LD50 of 2.78.upsilon.M in cytotoxicity assay.
- ST **arylchlorin** dihydroxy prepn phototoxicity cytotoxicity; **metallodihydroxyarylchlorins** phototoxicity cytotoxicity; **bacteriochlorin** aryl tetrahydroxy prepn phototoxicity cytotoxicity; photosensitizer photodynamic therapy; **tetraarylporphyrin** stereoselective dihydroxylation osmium tetroxide
- IT **Porphyrins**  
 RL: ADV (Adverse effect, including toxicity); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (.chlorins, metallo-; synthesis of .beta.,.beta.,-dihydroxymeso-substituted **chlorins**, **isobacteriochlorins**, and **bacteriochlorins** with improved photosensitizer activity)
- IT Dihydroxylation  
 (stereoselective, osmium tetroxide; synthesis of .beta.,.beta.,-dihydroxymeso-substituted **chlorins**, **isobacteriochlorins**, and **bacteriochlorins** with improved photosensitizer activity)
- IT Photodynamic therapy  
 Photosensitizers (pharmaceutical)  
 Phototoxicity  
 (synthesis of .beta.,.beta.,-dihydroxymeso-substituted **chlorins**, **isobacteriochlorins**, and **bacteriochlorins** with improved photosensitizer activity)
- IT 51552-53-5P 165336-18-5P 165336-21-0P 172925-98-3P 301336-58-3P  
 301336-61-8P 301336-66-3P 301336-70-9P 301336-74-3P 301336-78-7P  
 301336-82-3P 301336-85-6P 301336-88-9P 301336-91-4P 301336-94-7P  
 301336-97-0P 301337-00-8P 301337-03-1P 301337-05-3P 301337-07-5P  
 301337-10-0P 301337-13-3P 301337-16-6P **301337-19-9P**  
 301337-23-5P 301338-12-5P 301530-01-8P 301530-02-9P 301530-03-0P  
 RL: ADV (Adverse effect, including toxicity); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study);



PREP (Preparation); USES (Uses)  
(synthesis of .beta.,.beta.,-dihydroxymeso-substituted **chlorins**  
, **isobacteriochlorins**, and **bacteriochlorins** with  
improved photosensitizer activity)

IT 7429-90-5P, Aluminum, preparation 7440-21-3P, Silicon, preparation  
7440-26-8P, Technetium, preparation 7440-31-5P, Tin, preparation  
7440-55-3P, Gallium, preparation 7440-56-4P, Germanium, preparation  
7440-66-6P, Zinc, preparation 7440-74-6P, Indium, preparation  
14546-48-6P, Manganese(III), preparation 14701-22-5P, Nickel(II),  
preparation 15158-11-9P, Copper(II), preparation 22541-19-1P,  
Gadolinium, ion(3+), preparation  
RL: BAC (Biological activity or effector, except adverse); BSU (Biological  
study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);  
BIOL (Biological study); PREP (Preparation); USES (Uses)  
(synthesis of .beta.,.beta.,-dihydroxymeso-substituted **chlorins**  
, **isobacteriochlorins**, and **bacteriochlorins** with  
improved photosensitizer activity)

IT 74-88-4, Methyl iodide, reactions 917-23-7, **Tetraphenylporphyrin**  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(synthesis of .beta.,.beta.,-dihydroxymeso-substituted **chlorins**  
, **isobacteriochlorins**, and **bacteriochlorins** with  
improved photosensitizer activity)

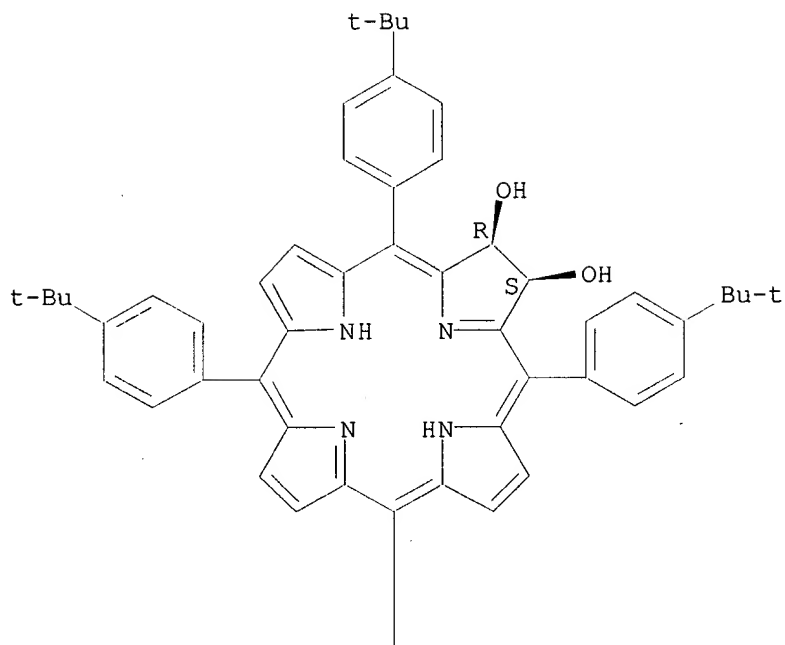
RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD  
RE  
(1) Dolphin; US 5684485 A 1997  
(2) Univ British Columbia; WO 9613504 A 1996 HCAPLUS

IT **301337-19-9P**  
RL: ADV (Adverse effect, including toxicity); BAC (Biological activity or  
effector, except adverse); BSU (Biological study, unclassified); SPN  
(Synthetic preparation); THU (Therapeutic use); BIOL (Biological study);  
PREP (Preparation); USES (Uses)  
(synthesis of .beta.,.beta.,-dihydroxymeso-substituted **chlorins**  
, **isobacteriochlorins**, and **bacteriochlorins** with  
improved photosensitizer activity)

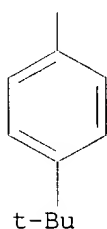
RN 301337-19-9 HCAPLUS  
CN 21H,23H-Porphine-7,8-diol, 5,10,15,20-tetrakis[4-(1,1-  
dimethylethyl)phenyl]-7,8-dihydro-, (7R,8S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A



PAGE 2-A



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L57 ANSWER 1 OF 8 HCAPLUS COPYRIGHT 2002 ACS  
 AN 2002:134544 HCAPLUS  
 DN 136:321357  
 TI Porphyrin, Chlorin, and Bacteriochlorin Isothiocyanates: Useful Reagents for the Synthesis of Photoactive Bioconjugates  
 AU Sutton, J. M.; Clarke, O. J.; Fernandez, N.; Boyle, R. W.  
 CS Department of Biological Sciences, University of Essex, Colchester, CO4 3SQ, UK  
 SO Bioconjugate Chemistry (2002), 13(2), 249-263  
 CODEN: BCCHEs; ISSN: 1043-1802  
 PB American Chemical Society  
 DT Journal  
 LA English  
 CC 8-9 (Radiation Biochemistry)  
 Section cross-reference(s): 9, 26  
 AB A novel method for conjugating porphyrins and related mols. to proteins has been developed. The method, which involves synthesizing porphyrins,

chlorins, and bacteriochlorins bearing a single amine-reactive isothiocyanate group represents a facile system for protein labeling with these photoactive species. Problems assocd. with the noncovalent binding of porphyrins to proteins are highlighted, and a method for purifying conjugates to yield exclusively covalently bound porphyrin protein species is demonstrated. Biol. activity of porphyrin-bovine serum albumin conjugates formed and purified by these methods is demonstrated using laser scanning confocal microscopy.

- ST porphyrin protein conjugate prepn carcinoma uptake  
 IT Functional groups  
     (isothiocyanato group; porphyrin-protein conjugate prepn. and tumor uptake)  
 IT Carcinoma  
     Conjugation (bond)  
     Fluorescence  
     Fluorescent indicators  
     Human  
     Microscopy  
     (porphyrin-protein conjugate prepn. and tumor uptake)  
 IT **Porphyrins**  
     RL: DGN (Diagnostic use); PKT (Pharmacokinetics); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
     (protein conjugates; porphyrin-protein conjugate prepn. and tumor uptake)  
 IT Albumins, biological studies  
     RL: DGN (Diagnostic use); PKT (Pharmacokinetics); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
     (serum, porphyrin conjugates; porphyrin-protein conjugate prepn. and tumor uptake)  
 IT 385384-58-7P 385384-59-8P 414866-60-7P 414866-61-8P  
     RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)  
     (porphyrin-protein conjugate prepn. and tumor uptake)  
 IT 2683-78-5DP, BacterioChlorin, derivs., protein conjugates 2683-84-3DP, Chlorin, derivs., protein conjugates  
     RL: DGN (Diagnostic use); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
     (porphyrin-protein conjugate prepn. and tumor uptake)  
 IT **318488-18-5P 385384-43-0P**  
     RL: PUR (Purification or recovery); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
     (porphyrin-protein conjugate prepn. and tumor uptake)  
 IT 176446-62-1 214554-43-5 367277-50-7  
     RL: RCT (Reactant); RACT (Reactant or reagent)  
     (porphyrin-protein conjugate prepn. and tumor uptake)  
 IT 127800-97-9P 154960-65-3P 155165-82-5P 250764-51-3P 250764-53-5P  
     253666-30-7P 253666-33-0P 253666-35-2P 253666-41-0P 253666-46-5P  
     318488-31-2P 385384-40-7P 385384-44-1P 385384-48-5P 385384-50-9P  
     385384-52-1P 385384-54-3P 385384-75-8P 414866-48-1P 414866-49-2P  
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     414866-55-0P 414866-56-1P 414866-57-2P 414866-58-3P 414866-59-4P  
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
     (porphyrin-protein conjugate prepn. and tumor uptake)  
 RE.CNT 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD  
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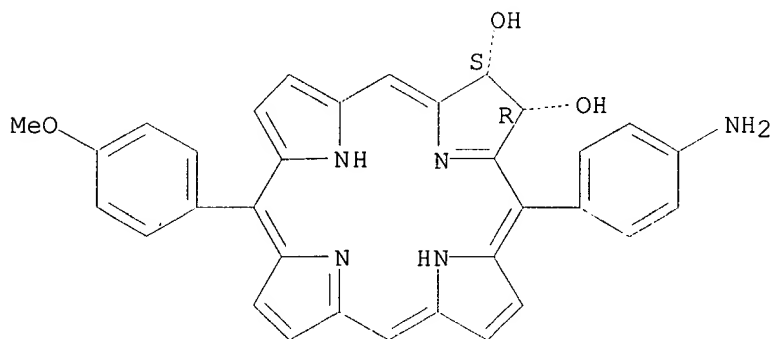
IT 318488-18-5P 385384-43-0P

RL: PUR (Purification or recovery); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(porphyrin-protein conjugate prepn. and tumor uptake)

RN 318488-18-5 HCAPLUS

CN 21H,23H-Porphine-7,8-diol, 5-(4-aminophenyl)-7,8-dihydro-15-(4-methoxyphenyl)-, (7R,8S)-rel- (9CI) (CA INDEX NAME)

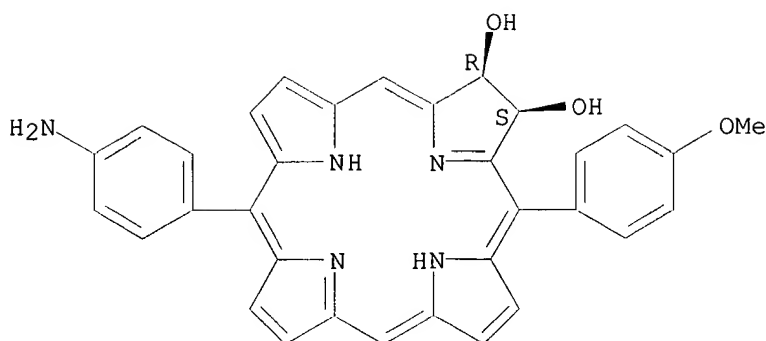
Relative stereochemistry.



RN 385384-43-0 HCAPLUS

CN 21H,23H-Porphine-7,8-diol, 15-(4-aminophenyl)-7,8-dihydro-5-(4-methoxyphenyl)-, (7R,8S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L57 ANSWER 2 OF 8 HCAPLUS COPYRIGHT 2002 ACS

AN 2002:10481 HCAPLUS

DN 136:69694

TI Preparation of novel porphyrin and porphyrin-based chromophores which may be particularly useful in a range of photodynamic applications

IN Boyle, Ross William; Clarke, Oliver James; Sutton, Jonathan Mark; Greenman, John

PA Catalyst Biomedica Ltd., UK

SO PCT Int. Appl., 128 pp.

CODEN: PIXXD2

DT Patent

LA English

IC ICM C07D487-22

ICS C09K009-02; A61K031-40

CC 26-4 (Biomolecules and Their Synthetic Analogs)

Section cross-reference(s): 63, 74

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2002000662	A1	20020103	WO 2001-GB2846	20010626 <--
	W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
	RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
	AU 2001070748	A5	20020108	AU 2001-70748	20010626 <--
PRAI	US 2000-214075P	P	20000626 <--		
	GB 2001-13784	A	20010606		
	WO 2001-GB2846	W	20010626		
OS	MARPAT 136:69694				
GI					

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB The present invention relates to the prepn. of novel porphyrins of formula I [R1 = aryl moiety linked to a conjugating group which is capable of conjugating the chromophore to a polypeptide mol. for delivering said chromophore to a specific biol. target in vitro or in vivo; R2 = hydrophilic aryl; R3 = H, hydrophilic aryl, or hydrophilic non-arom. moiety] and related chlorin and bacteriochlorin chromophores and sets of

- porphyrin and porphyrin-based chromophores, which may be particularly useful in a range of photodynamic applications, including photochemotherapy and fluorescence anal. and imaging (no data). Thus, 4-acetamidobenzaldehyde and 3,5-dimethoxybenzaldehyde were stirred in propionic acid and treated with pyrrole to afford 5-(4-acetamidophenyl)-10,15,20-tris(3,5-dimethoxyphenyl)porphyrin (II) in 9.1%.
- ST porphyrin chlorin bacteriochlorin chromophore prepn photochemotherapy fluorescence analysis imaging
- IT Gel electrophoresis  
(SDS; elution of porphyrin-antibody bioconjugates from SDS PAGE utilizing micro-electroeluter)
- IT Cytometry  
(flow; prepn. of novel porphyrin and porphyrin-based chromophores which may be particularly useful in a range of photodynamic applications)
- IT AIDS (disease)  
Autoimmune disease  
Multiple sclerosis  
Rheumatoid arthritis  
(method for treating a disease or disorder which is characterized by the presence in the body of diseased or undesired cells, such as)
- IT Cytotoxicity  
(photo-; prepn. of novel porphyrin and porphyrin-based chromophores which may be particularly useful in a range of photodynamic applications)
- IT Confocal laser scanning microscopy  
Photodynamic therapy  
(prepn. of novel porphyrin and porphyrin-based chromophores which may be particularly useful in a range of photodynamic applications)
- IT Suzuki coupling reaction  
(prepn. of novel porphyrin and porphyrin-based chromophores which may be particularly useful in a range of photodynamic applications via)
- IT 253666-30-7P 253666-33-0P 268737-71-9P **318488-18-5P**  
**385384-43-0P** 385384-44-1P 385384-45-2P 385384-46-3P  
385384-48-5P 385384-49-6P 385384-50-9P 385384-51-0P  
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)  
(prepn. of novel porphyrin and porphyrin-based chromophores which may be particularly useful in a range of photodynamic applications)
- IT 253666-35-2P **318488-06-1P** 385384-47-4P 385384-52-1P  
385384-53-2P 385384-54-3P 385384-55-4P 385384-56-5P 385384-57-6P  
385384-58-7P 385384-59-8P **385384-60-1P** 385384-61-2P  
385384-62-3P 385384-63-4P 385384-64-5P 385384-65-6P 385384-66-7P  
385384-67-8P 385384-68-9P 385384-69-0P 385384-70-3P 385384-71-4P  
385384-72-5P 385384-73-6P 385384-74-7P 385384-75-8P 385384-76-9P  
385384-77-0P 385384-79-2P 385384-83-8P 385384-84-9P 385384-85-0P  
385384-86-1P 385384-87-2P  
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(prepn. of novel porphyrin and porphyrin-based chromophores which may be particularly useful in a range of photodynamic applications)
- IT 86-81-7, 3,4,5-Trimethoxybenzaldehyde 109-97-7, Pyrrole 122-85-0,  
4-Acetamidobenzaldehyde 123-11-5, reactions 500-22-1,  
3-Pyridinecarboxaldehyde 872-85-5, 4-Pyridinecarboxaldehyde 7311-34-4,  
3,5-Dimethoxybenzaldehyde 28920-43-6, 9-Fluorenylmethyl chloroformate  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(prepn. of novel porphyrin and porphyrin-based chromophores which may be particularly useful in a range of photodynamic applications)
- IT 127800-97-9P 154960-65-3P 167482-90-8P 176446-62-1P 214554-43-5P  
250764-51-3P 250764-53-5P 385384-40-7P 385384-41-8P 385384-42-9P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of novel porphyrin and porphyrin-based chromophores which may be particularly useful in a range of photodynamic applications)

RE.CNT 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD

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IT 318488-18-5P 385384-43-0P

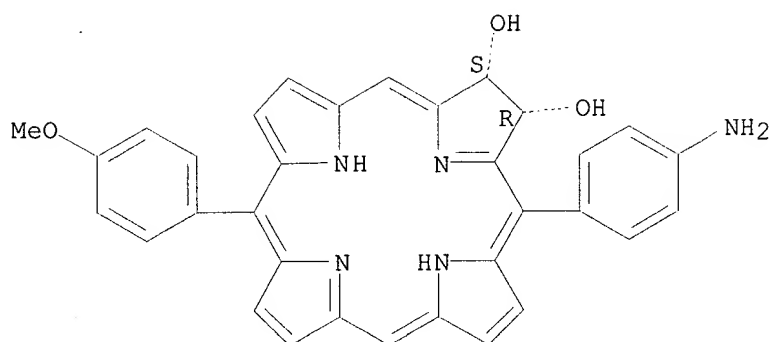
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(prepn. of novel porphyrin and porphyrin-based chromophores which may be particularly useful in a range of photodynamic applications)

RN 318488-18-5 HCAPLUS

CN 21H,23H-Porphine-7,8-diol, 5-(4-aminophenyl)-7,8-dihydro-15-(4-methoxyphenyl)-, (7R,8S)-rel- (9CI) (CA INDEX NAME)

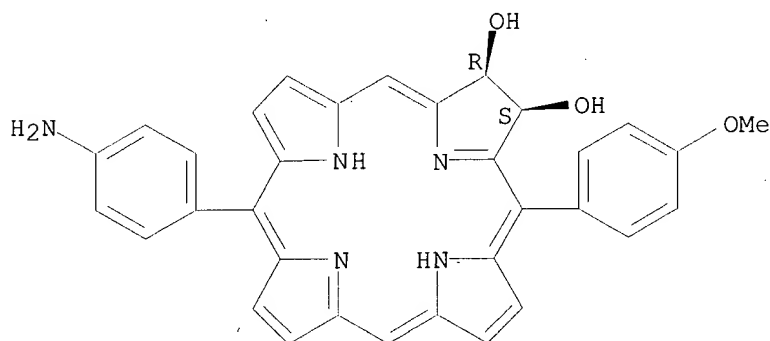
Relative stereochemistry.



RN 385384-43-0 HCAPLUS

CN 21H,23H-Porphine-7,8-diol, 15-(4-aminophenyl)-7,8-dihydro-5-(4-methoxyphenyl)-, (7R,8S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



IT 318488-06-1P 385384-60-1P

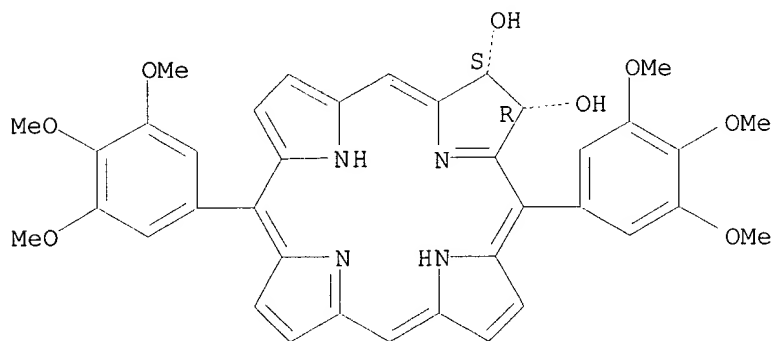
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of novel porphyrin and porphyrin-based chromophores which may be particularly useful in a range of photodynamic applications)

RN 318488-06-1 HCAPLUS

CN 21H,23H-Porphine-7,8-diol, 7,8-dihydro-5,15-bis(3,4,5-trimethoxyphenyl)-, (7R,8S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

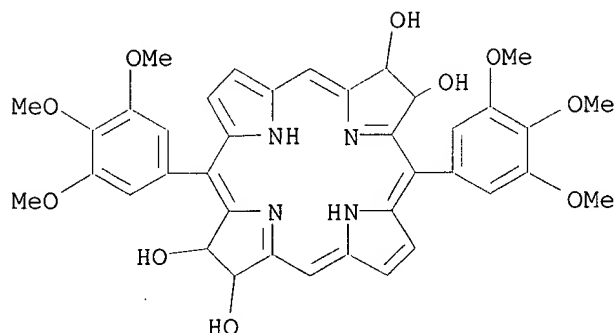


RN 385384-60-1 HCAPLUS

CN 21H,23H-Porphine-7,8,17,18-tetrol, 7,8,17,18-tetrahydro-5,15-bis(3,4,5-



trimethoxyphenyl)- (9CI) (CA INDEX NAME)



- L57 ANSWER 3 OF 8 HCAPLUS COPYRIGHT 2002 ACS  
 AN 2000:831421 HCAPLUS  
 DN 134:100684  
 TI Functionalized diphenylchlorins and bacteriochlorins: their synthesis and bioconjugation for targeted photodynamic therapy and tumor cell imaging  
 AU Sutton, Jonathan M.; Fernandez, Nelson; Boyle, Ross W.  
 CS Department of Biological Sciences, University of Essex, Colchester, CO4 3SQ, UK  
 SO Journal of Porphyrins and Phthalocyanines (2000), 4(7), 655-658  
 CODEN: JPPHFZ; ISSN: 1088-4246  
 PB John Wiley & Sons Ltd.  
 DT Journal  
 LA English  
 CC 26-7 (Biomolecules and Their Synthetic Analogs)  
 Section cross-reference(s): 9, 22  
 OS CASREACT 134:100684  
 AB A range of 5,15-diphenylporphyrins with sym. and unsym. substitution patterns were subjected to osmium tetroxide-mediated dihydroxylations. The resulting chlorins and bacteriochlorins present an important group of compds. for studying structure-activity relationships of photodynamic sensitizers. The regioselectivity of the dihydroxylation of various 5,15-diphenylporphyrins with unsym. substitution patterns was also examd. Both diphenylchlorin diol (DPC) and diphenylbacteriochlorin tetrol (DPBC) examples were converted into reactive isothiocyanates and conjugated with bovine serum albumin (BSA).  
 ST porphyrin diphenyl dihydroxylation regioselective; chlorin diphenyl dihydroxy tetrahydroxy prepn; diphenylchlorin bacteriochlorin isothiocyanate conjugate BSA  
 IT **Porphyrins**  
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (chlorins, di-Ph; synthesis and bioconjugation of functionalized diphenylchlorins and bacteriochlorins for targeted photodynamic therapy and tumor cell imaging)  
 IT Albumins, biological studies  
 RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process) (conjugates; synthesis and bioconjugation of functionalized diphenylchlorins and bacteriochlorins for targeted photodynamic therapy and tumor cell imaging)  
 IT Dihydroxylation  
 (stereoselective; synthesis and bioconjugation of functionalized diphenylchlorins and bacteriochlorins for targeted photodynamic therapy and tumor cell imaging)  
 IT Fluorescence  
 UV and visible spectra

(synthesis and bioconjugation of functionalized diphenylchlorins and bacteriochlorins for targeted photodynamic therapy and tumor cell imaging)

IT 318488-18-5P 318488-24-3P  
 RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (synthesis and bioconjugation of functionalized diphenylchlorins and bacteriochlorins for targeted photodynamic therapy and tumor cell imaging)

IT 318488-06-1P 318488-12-9P 318488-23-2P  
 318488-29-8P 318488-30-1DP, conjugate with BSA 318488-31-2DP, conjugate with BSA  
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
 (synthesis and bioconjugation of functionalized diphenylchlorins and bacteriochlorins for targeted photodynamic therapy and tumor cell imaging)

IT 22112-89-6, 5,15-Diphenylporphyrin 128374-05-0 253666-33-0  
 268737-71-9 318488-01-6 318488-02-7 318488-13-0 318488-14-1  
 318488-15-2 318488-16-3 318488-17-4  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (synthesis and bioconjugation of functionalized diphenylchlorins and bacteriochlorins for targeted photodynamic therapy and tumor cell imaging)

IT 165336-21-0P 318488-03-8P 318488-04-9P 318488-05-0P  
 318488-07-2P 318488-08-3P 318488-10-7P 318488-11-8P  
 318488-19-6P 318488-20-9P 318488-21-0P  
 318488-22-1P 318488-25-4P 318488-26-5P  
 318488-27-6P 318488-28-7P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (synthesis and bioconjugation of functionalized diphenylchlorins and bacteriochlorins for targeted photodynamic therapy and tumor cell imaging)

RE.CNT 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

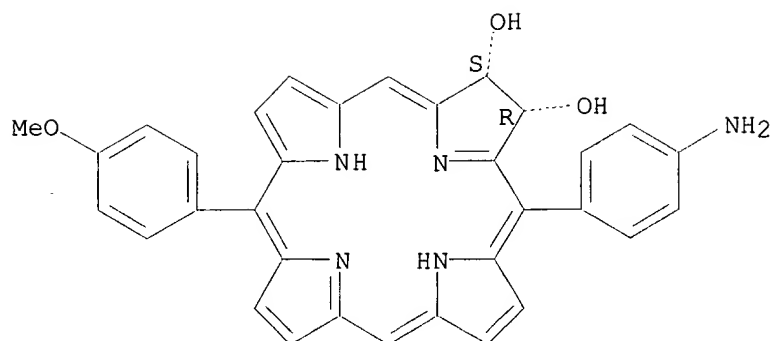
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IT 318488-18-5P 318488-24-3P  
 RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (synthesis and bioconjugation of functionalized diphenylchlorins and bacteriochlorins for targeted photodynamic therapy and tumor cell imaging)

RN 318488-18-5 HCAPLUS

CN 21H,23H-Porphine-7,8-diol, 5-(4-aminophenyl)-7,8-dihydro-15-(4-methoxyphenyl)-, (7R,8S)-rel- (9CI) (CA INDEX NAME)

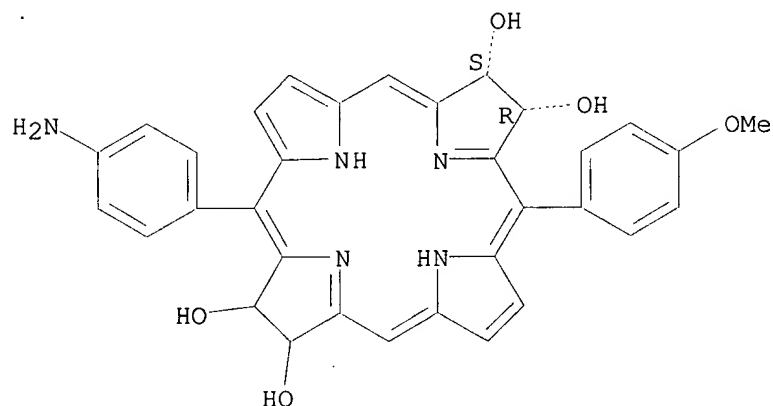
Relative stereochemistry.



RN 318488-24-3 HCAPLUS

CN 21H,23H-Porphine-7,8,17,18-tetrol, 5-(4-aminophenyl)-7,8,17,18-tetrahydro-15-(4-methoxyphenyl)-, (17R,18S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



IT 318488-06-1P 318488-12-9P 318488-23-2P

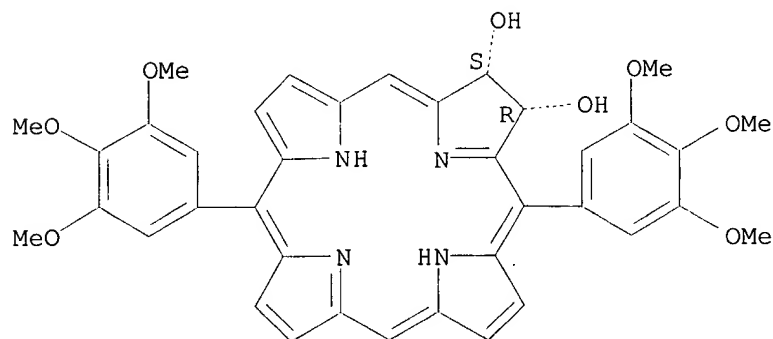
318488-29-8P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
(synthesis and bioconjugation of functionalized diphenylchlorins and bacteriochlorins for targeted photodynamic therapy and tumor cell imaging)

RN 318488-06-1 HCAPLUS

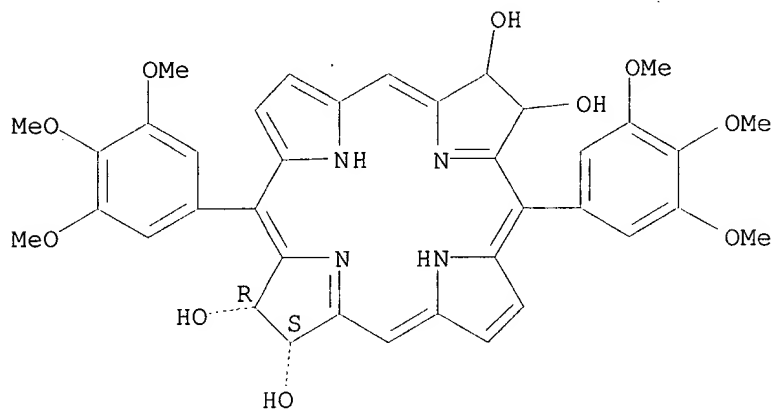
CN 21H,23H-Porphine-7,8-diol, 7,8-dihydro-5,15-bis(3,4,5-trimethoxyphenyl)-, (7R,8S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



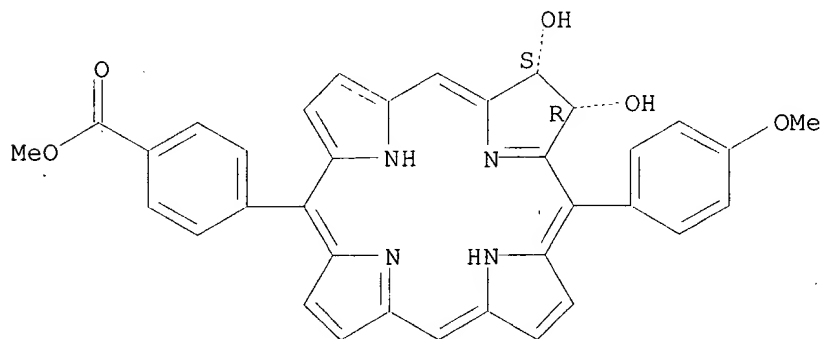
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Relative stereochemistry.



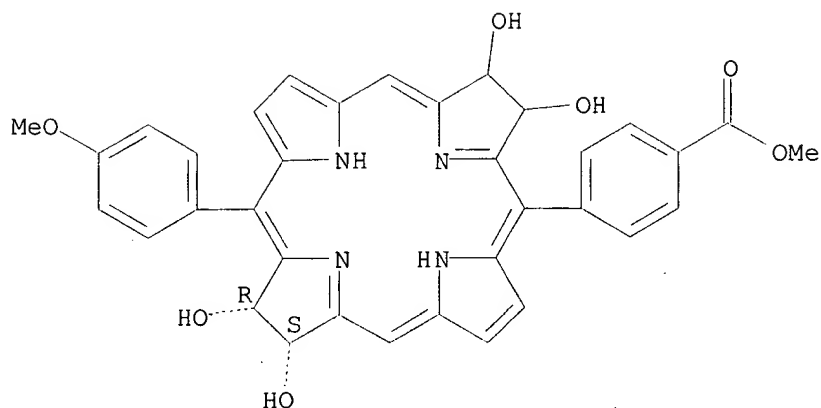
RN 318488-23-2 HCAPLUS  
 CN Benzoic acid, 4-[(17R,18S)-17,18-dihydro-17,18-dihydroxy-15-(4-methoxyphenyl)-21H,23H-porphin-5-yl]-, methyl ester, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry..



RN 318488-29-8 HCAPLUS  
 CN Benzoic acid, 4-[(17R,18S)-7,8,17,18-tetrahydro-7,8,17,18-tetrahydroxy-15-(4-methoxyphenyl)-21H,23H-porphin-5-yl]-, methyl ester, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



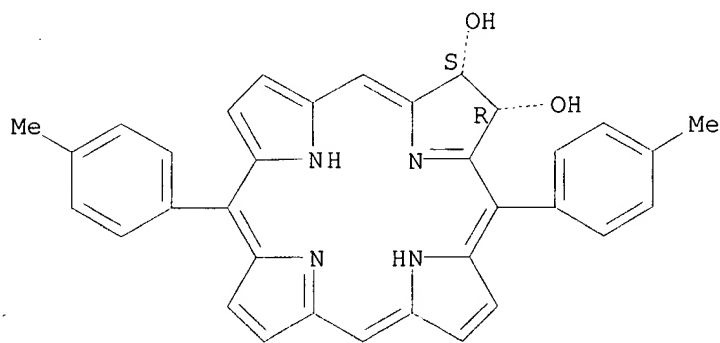
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 318488-21-0P 318488-22-1P 318488-25-4P  
 318488-26-5P 318488-27-6P 318488-28-7P

RL: SPN (Synthetic preparation); PREP (Preparation)  
 (synthesis and bioconjugation of functionalized diphenylchlorins and  
 bacteriochlorins for targeted photodynamic therapy and tumor cell  
 imaging)

RN 318488-03-8 HCAPLUS

CN 21H,23H-Porphine-7,8-diol, 7,8-dihydro-5,15-bis(4-methylphenyl)-,  
 (7R,8S)-rel- (9CI) (CA INDEX NAME)

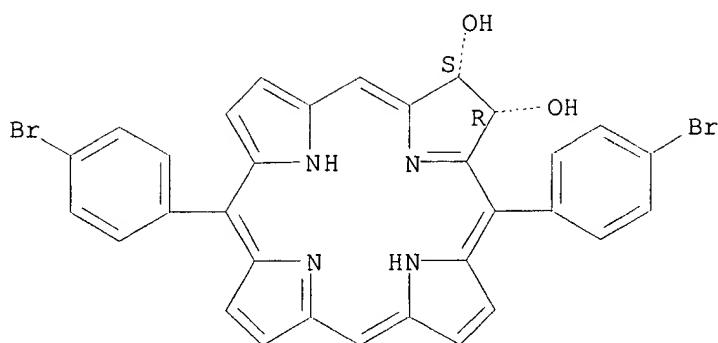
Relative stereochemistry.



RN 318488-04-9 HCAPLUS

CN 21H,23H-Porphine-7,8-diol, 5,15-bis(4-bromophenyl)-7,8-dihydro-,  
 (7R,8S)-rel- (9CI) (CA INDEX NAME)

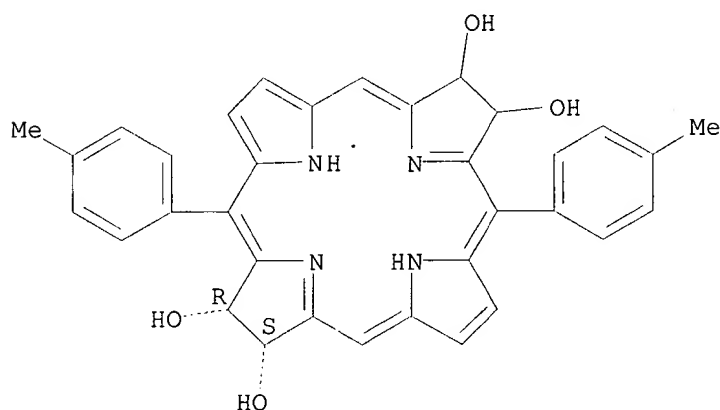
Relative stereochemistry.



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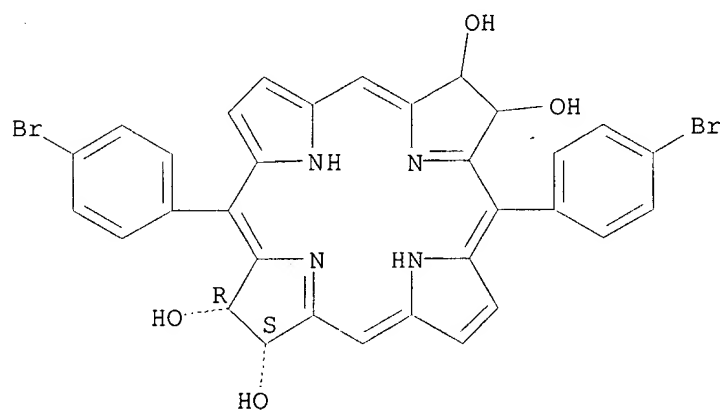
Relative stereochemistry.



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Relative stereochemistry.

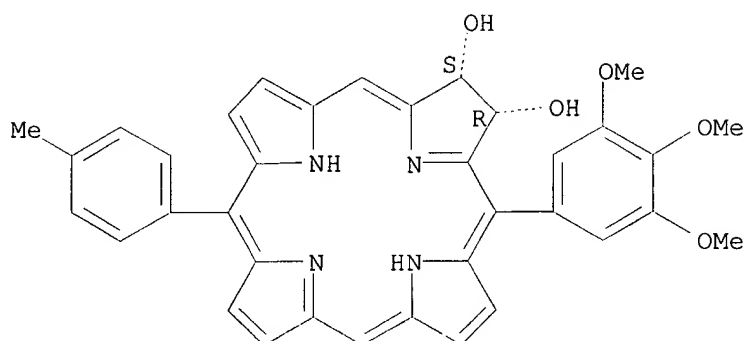


RN 318488-19-6 HCAPLUS

CN 21H,23H-Porphine-7,8-diol, 7,8-dihydro-15-(4-methylphenyl)-5-(3,4,5-tribromophenyl)-, (7R,8S)-rel- (9CI) (CA INDEX NAME)

trimethoxyphenyl)-, (7R,8S)-rel- (9CI) (CA INDEX NAME)

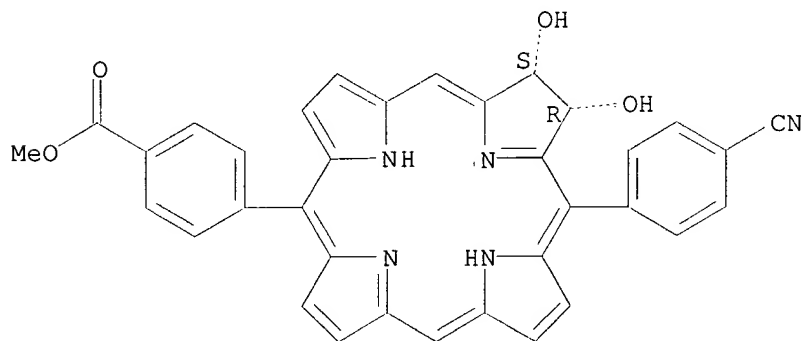
Relative stereochemistry.



RN 318488-20-9 HCAPLUS

CN Benzoic acid, 4-[(17R,18S)-15-(4-cyanophenyl)-17,18-dihydro-17,18-dihydroxy-21H,23H-porphin-5-yl]-, methyl ester, rel- (9CI) (CA INDEX NAME)

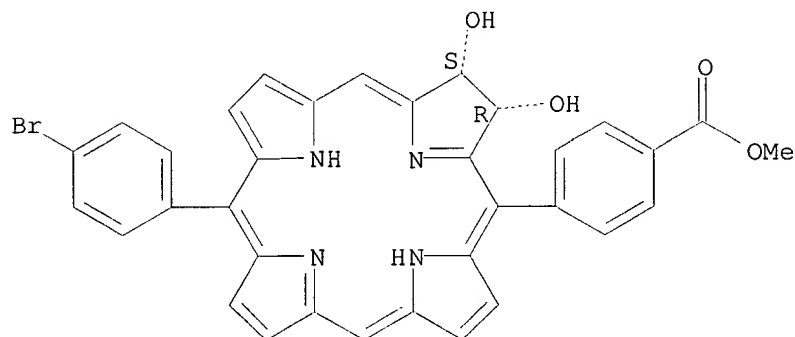
Relative stereochemistry.



RN 318488-21-0 HCAPLUS

CN Benzoic acid, 4-[(7R,8S)-15-(4-bromophenyl)-7,8-dihydro-7,8-dihydroxy-21H,23H-porphin-5-yl]-, methyl ester, rel- (9CI) (CA INDEX NAME)

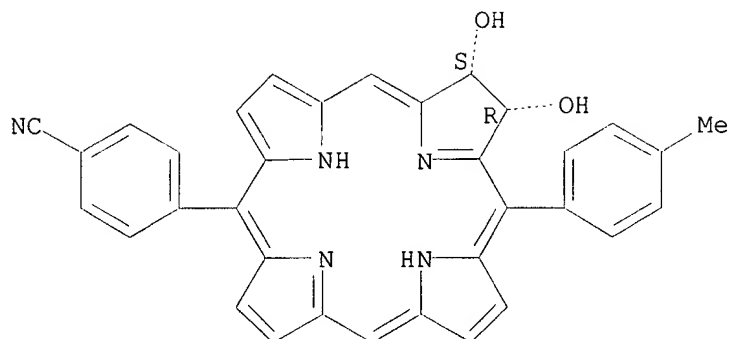
Relative stereochemistry.



RN 318488-22-1 HCAPLUS

CN Benzonitrile, 4-[(17R,18S)-17,18-dihydro-17,18-dihydroxy-15-(4-methylphenyl)-21H,23H-porphin-5-yl]-, rel- (9CI) (CA INDEX NAME)

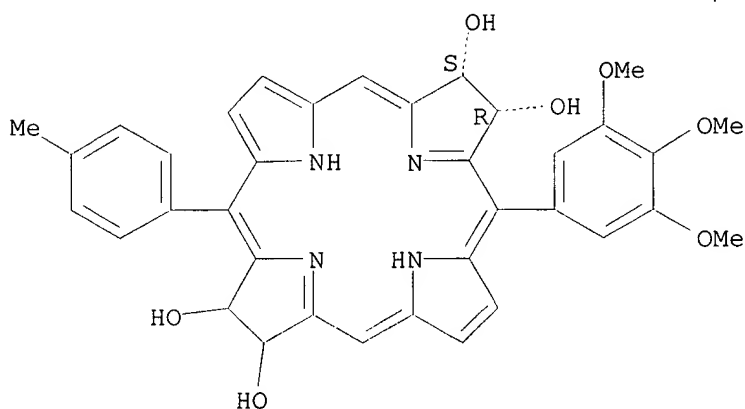
Relative stereochemistry.



RN 318488-25-4 HCAPLUS

CN 21H,23H-Porphine-7,8,17,18-tetrol, 7,8,17,18-tetrahydro-5-(4-methylphenyl)-15-(3,4,5-trimethoxyphenyl)-, (17R,18S)-rel- (9CI) (CA INDEX NAME)

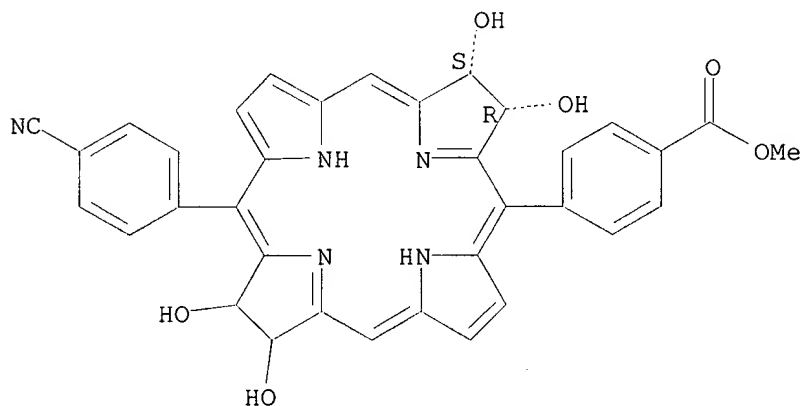
Relative stereochemistry.



RN 318488-26-5 HCAPLUS

CN Benzoic acid, 4-[(7R,8S)-15-(4-cyanophenyl)-7,8,17,18-tetrahydro-7,8,17,18-tetrahydroxy-21H,23H-porphin-5-yl]-, methyl ester, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

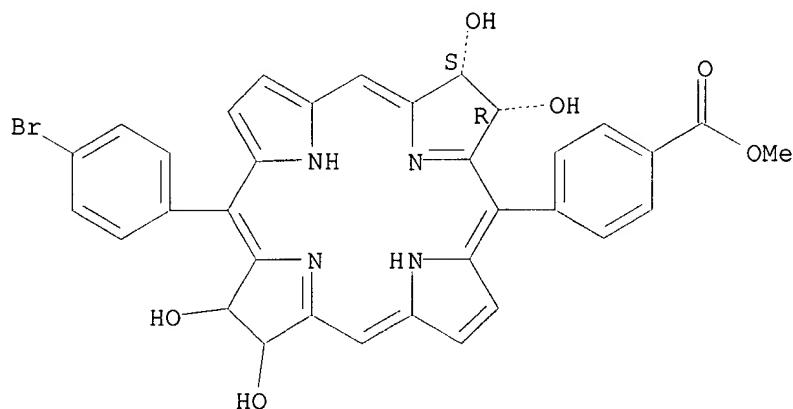




RN 318488-27-6 HCAPLUS

CN Benzoic acid, 4-[(7R,8S)-15-(4-bromophenyl)-7,8,17,18-tetrahydro-7,8,17,18-tetrahydroxy-21H,23H-porphin-5-yl]-, methyl ester, rel- (9CI) (CA INDEX NAME)

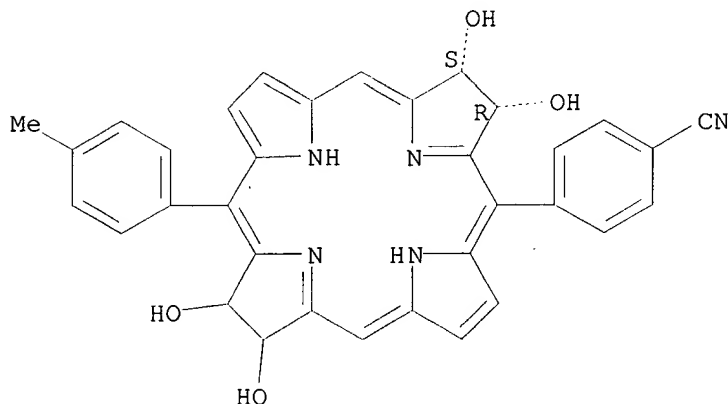
Relative stereochemistry.



RN 318488-28-7 HCAPLUS

CN Benzonitrile, 4-[(7R,8S)-7,8,17,18-tetrahydro-7,8,17,18-tetrahydroxy-15-(4-methylphenyl)-21H,23H-porphin-5-yl]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L57 ANSWER 4 OF 8 HCAPLUS COPYRIGHT 2002 ACS

AN 2000:742097 HCAPLUS

DN 133:296322

TI Synthesis of .beta.,.beta.,-dihydroxymeso-substituted **chlorins**, **isobacteriochlorins**, and **bacteriochlorins** with improved photosensitizer activity

IN Macalpine, Jill; Dolphin, David; Bruckner, Christian

PA University of British Columbia, Can.

SO PCT Int. Appl., 53 pp.

CODEN: PIXXD2

DT Patent

LA English

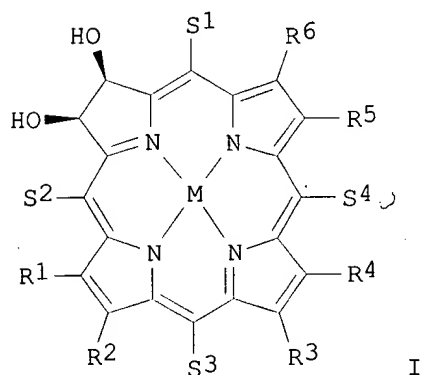
IC ICM C07D487-22

ICS A61K031-409; A61K049-00; A61P035-00; C07D487-22; C07D257-00;

C07D209-00; C07D209-00; C07D209-00; C07D209-00  
 CC 26-7 (Biomolecules and Their Synthetic Analogs)  
 Section cross-reference(s): 1, 8

FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2000061584	A1	20001019	WO 2000-CA435	20000414 <--
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
PRAI	US 1999-129324P	P	19990414 <--		
OS	MARPAT 133:296322				
GI					



AB Synthesis of .beta.,.beta.,-dihydroxymeso-substituted **chlorins** (I) [M = 2H, Ni(II), Cu(II), Zn, Sn, Ge, Si, Ga, Al, Mn(III), Gd(III), In, Tc; R1-R6 = independently H, alkyl, alkylcarboxylic acid or ester, =O, OH, NO2, NH2; taken together with another ring, ring substituent or meso substituent = fused 5- or 6-membered ring; S1-S4 independently = H, (un)substituted alkyl, (un)substituted aryl, (un)substituted cycloalkyl, may be same or different], **bacteriochlorins**, and **isobacteriochlorins** with improved photosensitizer activity is described. Thus, I (S1-S4 = Ph, M = 2H, R1-R6 = H) (II) is prepd. by treatment of **tetraphenylporphyrin** with osmium tetroxide. II shows an LD50 of 2.78.upsilon.M in cytotoxicity assay.

ST **arylchlorin** dihydroxy prepn phototoxicity cytotoxicity; **metallodihydroxyarylchlorins** phototoxicity cytotoxicity; **bacteriochlorin** aryl tetrahydroxy prepn phototoxicity cytotoxicity; photosensitizer photodynamic therapy; **tetraarylporphyrin** stereoselective dihydroxylation osmium tetroxide

IT **Porphyrins**  
 RL: ADV (Adverse effect, including toxicity); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (.chlorins, metallo-; synthesis of .beta.,.beta.,-dihydroxymeso-substituted **chlorins**,

**isobacteriochlorins**, and **bacteriochlorins** with improved photosensitizer activity)

IT Dihydroxylation  
(stereoselective, osmium tetroxide; synthesis of .beta.,.beta.,-dihydroxymeso-substituted **chlorins**, **isobacteriochlorins**, and **bacteriochlorins** with improved photosensitizer activity)

IT Photodynamic therapy  
Photosensitizers (pharmaceutical)  
Phototoxicity  
(synthesis of .beta.,.beta.,-dihydroxymeso-substituted **chlorins**, **isobacteriochlorins**, and **bacteriochlorins** with improved photosensitizer activity)

IT 51552-53-5P 165336-18-5P 165336-21-0P 172925-98-3P 301336-58-3P  
 301336-61-8P 301336-66-3P 301336-70-9P 301336-74-3P  
 301336-78-7P 301336-82-3P 301336-85-6P 301336-88-9P  
 301336-91-4P 301336-94-7P 301336-97-0P 301337-00-8P  
 301337-03-1P 301337-05-3P 301337-07-5P  
 301337-10-0P 301337-13-3P 301337-16-6P  
 301337-19-9P 301337-23-5P 301338-12-5P 301530-01-8P  
 301530-02-9P 301530-03-0P

RL: ADV (Adverse effect, including toxicity); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (synthesis of .beta.,.beta.,-dihydroxymeso-substituted **chlorins**, **isobacteriochlorins**, and **bacteriochlorins** with improved photosensitizer activity)

IT 7429-90-5P, Aluminum, preparation 7440-21-3P, Silicon, preparation  
 7440-26-8P, Technetium, preparation 7440-31-5P, Tin, preparation  
 7440-55-3P, Gallium, preparation 7440-56-4P, Germanium, preparation  
 7440-66-6P, Zinc, preparation 7440-74-6P, Indium, preparation  
 14546-48-6P, Manganese(III), preparation 14701-22-5P, Nickel(II), preparation 15158-11-9P, Copper(II), preparation 22541-19-1P, Gadolinium, ion(3+), preparation

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (synthesis of .beta.,.beta.,-dihydroxymeso-substituted **chlorins**, **isobacteriochlorins**, and **bacteriochlorins** with improved photosensitizer activity)

IT 74-88-4, Methyl iodide, reactions 917-23-7, **Tetraphenylporphyrin**  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (synthesis of .beta.,.beta.,-dihydroxymeso-substituted **chlorins**, **isobacteriochlorins**, and **bacteriochlorins** with improved photosensitizer activity)

RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE  
 (1) Dolphin; US 5684485 A 1997  
 (2) Univ British Columbia; WO 9613504 A 1996 HCAPLUS

IT 301336-61-8P 301336-74-3P 301336-78-7P  
 301336-88-9P 301336-91-4P 301337-00-8P  
 301337-03-1P 301337-07-5P 301337-10-0P  
 301337-13-3P 301337-16-6P 301337-23-5P  
 301530-01-8P 301530-02-9P 301530-03-0P

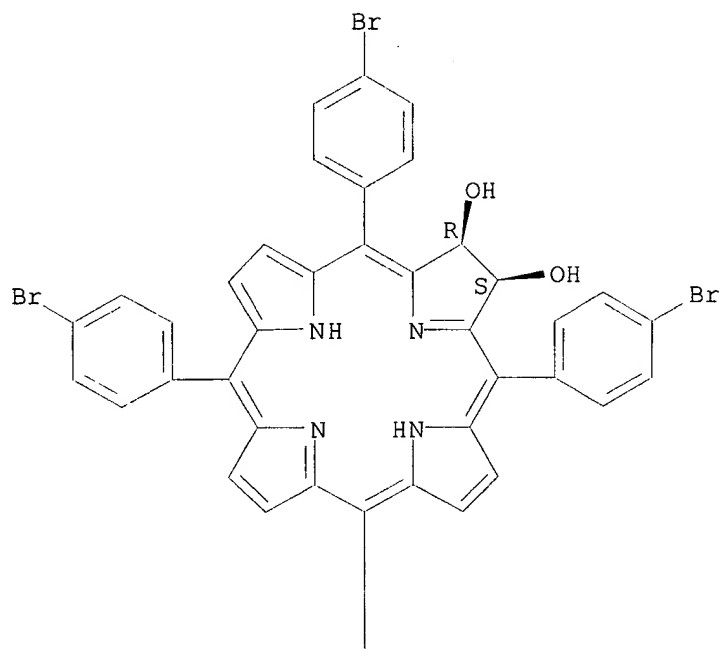
RL: ADV (Adverse effect, including toxicity); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (synthesis of .beta.,.beta.,-dihydroxymeso-substituted **chlorins**, **isobacteriochlorins**, and **bacteriochlorins** with improved photosensitizer activity)

RN 301336-61-8 HCAPLUS

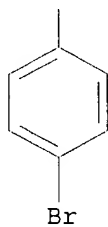
CN 21H,23H-Porphine-7,8-diol, 5,10,15,20-tetrakis(4-bromophenyl)-7,8-dihydro-  
, (7R,8S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A



PAGE 2-A

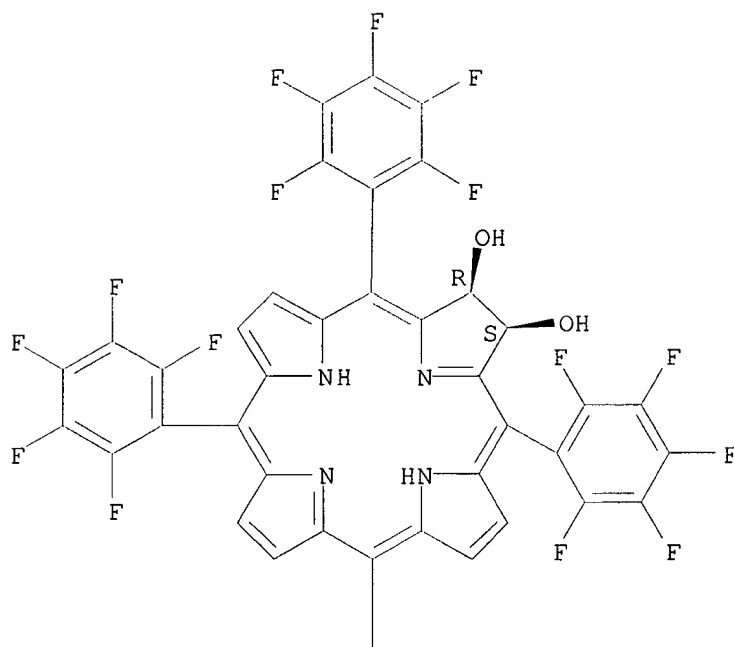


RN 301336-74-3 HCAPLUS

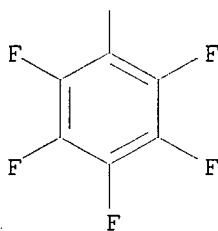
CN 21H,23H-Porphine-7,8-diol, 7,8-dihydro-5,10,15,20-  
tetrakis(pentafluorophenyl)-, (7R,8S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A



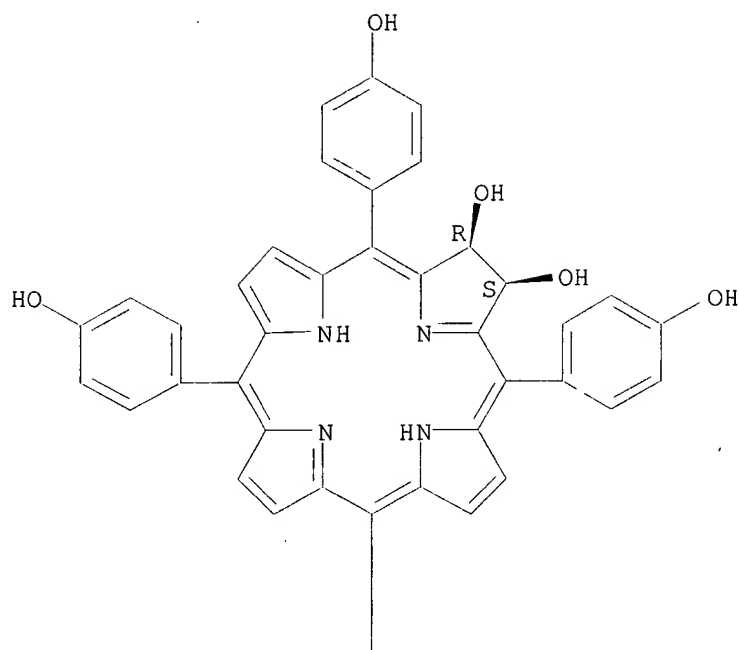
PAGE 2-A



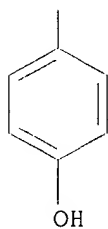
RN 301336-78-7 HCAPLUS  
CN 21H,23H-Porphine-7,8-diol, 7,8-dihydro-5,10,15,20-tetrakis(4-hydroxyphenyl)-, (7R,8S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A



PAGE 2-A

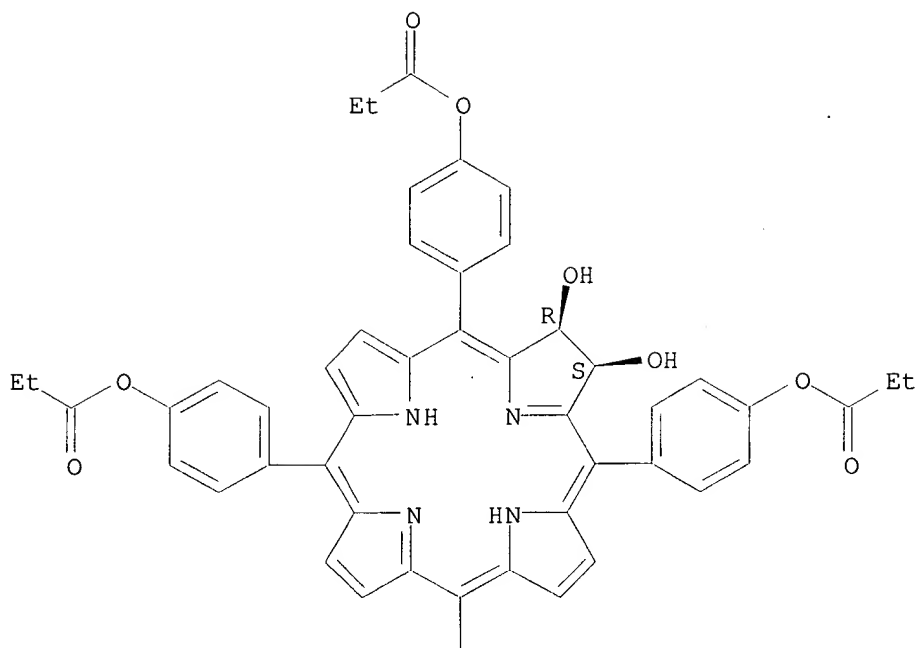


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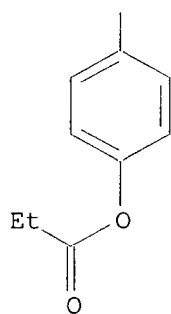
CN 21H,23H-Porphine-7,8-diol, 7,8-dihydro-5,10,15,20-tetrakis[4-(1-oxopropoxy)phenyl]-, (7R,8S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A



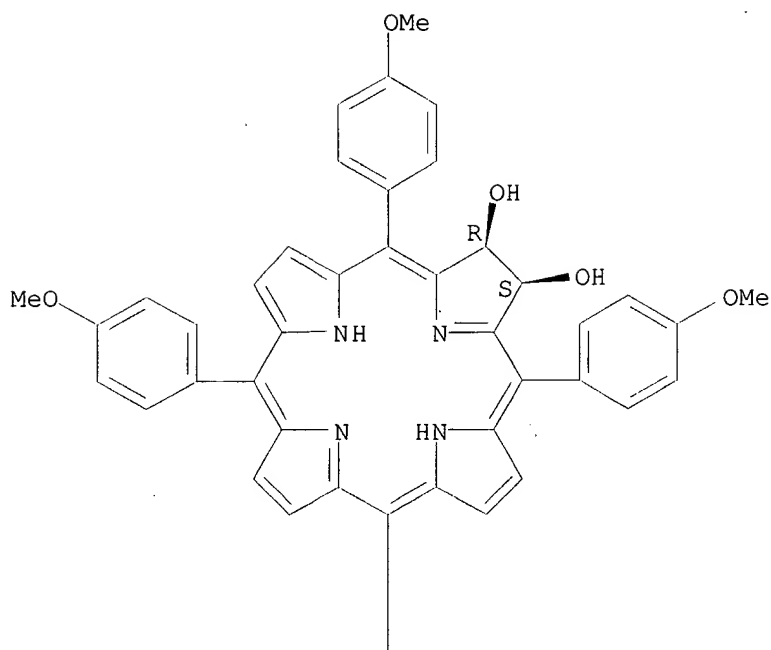
PAGE 2-A



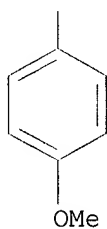
RN 301336-91-4 HCAPLUS  
CN 21H,23H-Porphine-7,8-diol, 7,8-dihydro-5,10,15,20-tetrakis(4-methoxyphenyl)-, (7R,8S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A



PAGE 2-A

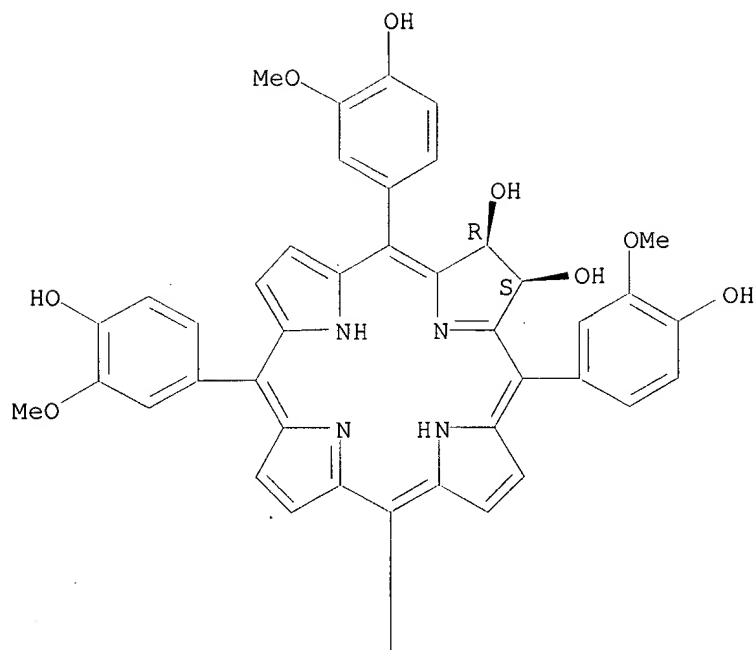


RN 301337-00-8 HCAPLUS  
CN 21H,23H-Porphine-7,8-diol, 7,8-dihydro-5,10,15,20-tetrakis(4-hydroxy-3-methoxyphenyl)-, (7R,8S)-rel- (9CI) (CA INDEX NAME)

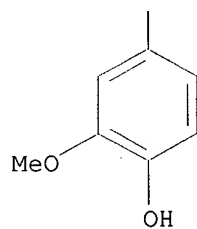
Relative stereochemistry.



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PAGE 2-A

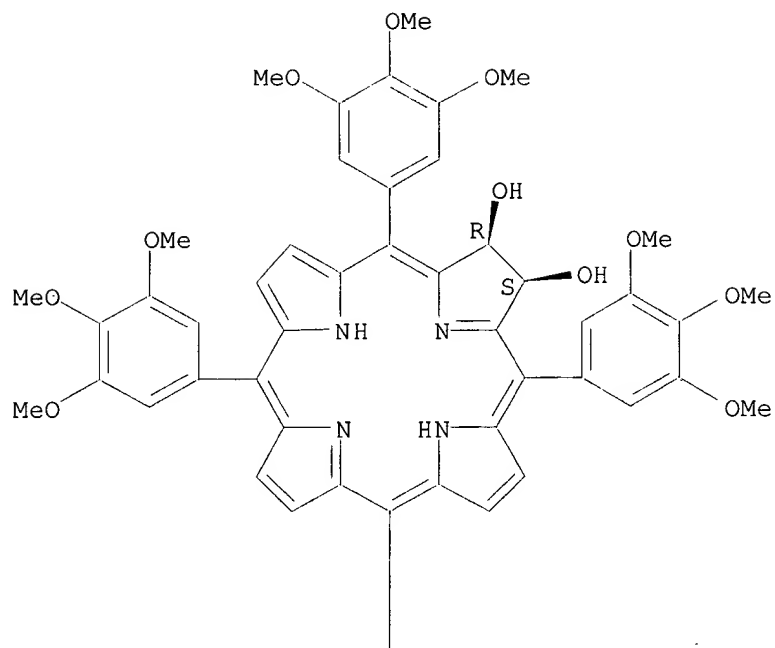


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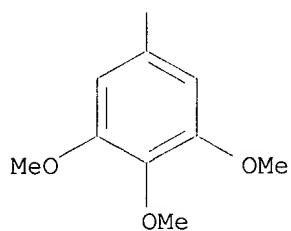
CN 21H,23H-Porphine-7,8-diol, 7,8-dihydro-5,10,15,20-tetrakis(3,4,5-trimethoxyphenyl)-, (7R,8S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

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PAGE 2-A

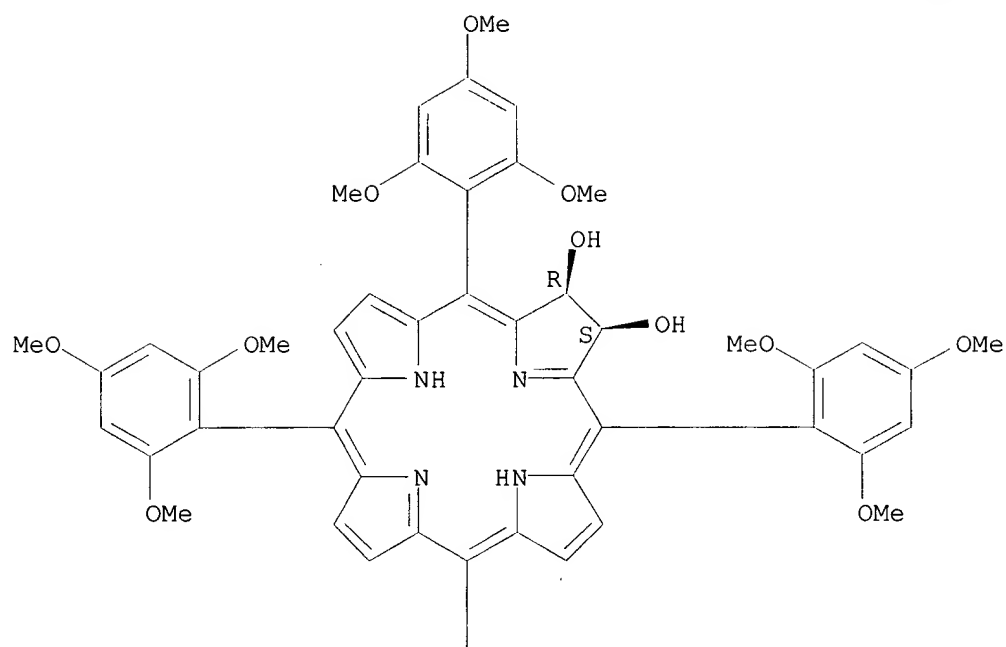


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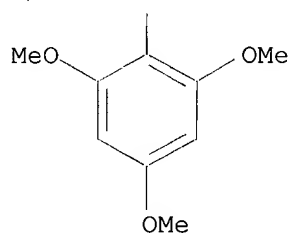
CN 21H,23H-Porphine-7,8-diol, 7,8-dihydro-5,10,15,20-tetrakis(2,4,6-trimethoxyphenyl)-, (7R,8S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

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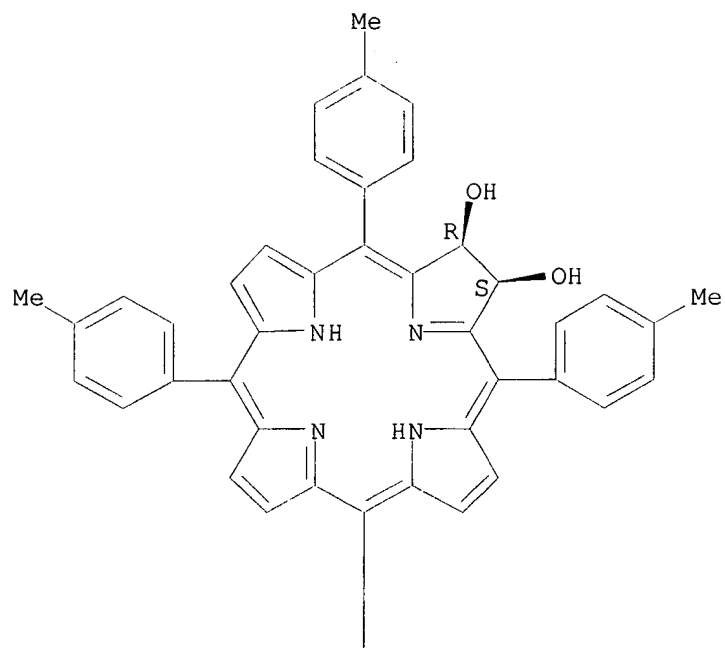


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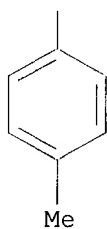
CN 21H,23H-Porphine-7,8-diol, 7,8-dihydro-5,10,15,20-tetrakis(4-methylphenyl)-  
, (7R,8S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A



PAGE 2-A

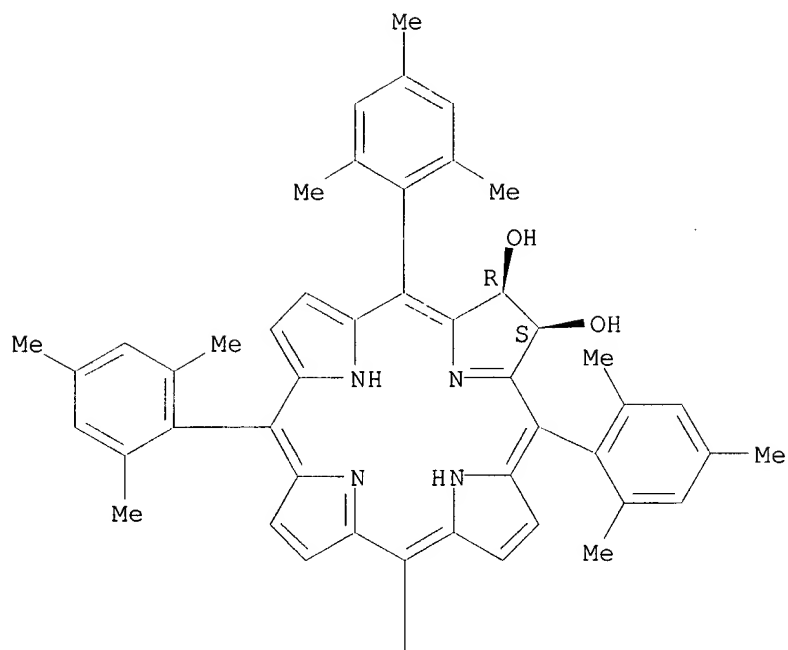


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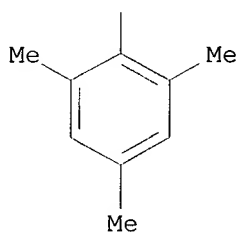
CN 21H,23H-Porphine-7,8-diol, 7,8-dihydro-5,10,15,20-tetrakis(2,4,6-trimethylphenyl)-, (7R,8S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A



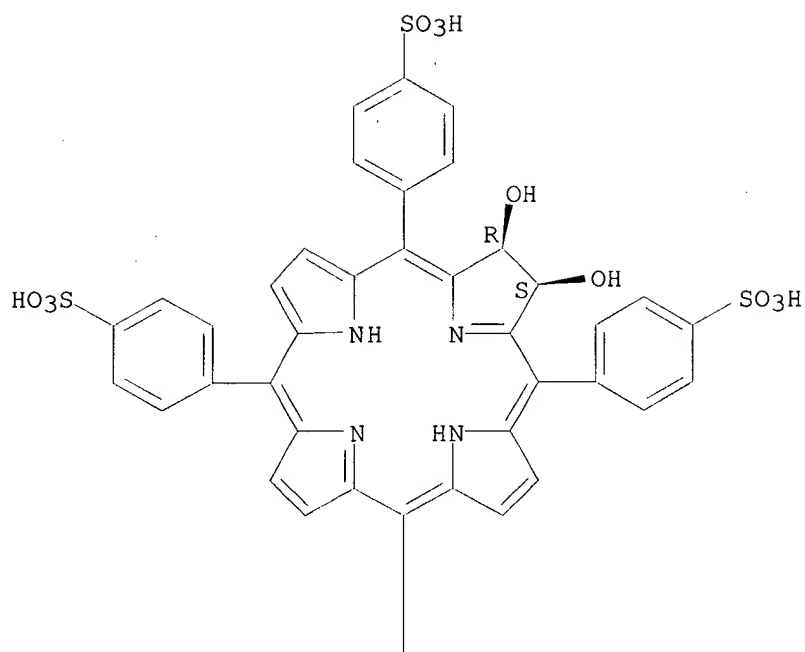
PAGE 2-A



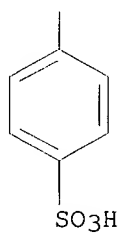
RN 301337-16-6 HCAPLUS  
 CN Benzenesulfonic acid, 4,4',4'',4'''-[(7R,8S)-7,8-dihydro-7,8-dihydroxy-21H,23H-porphine-5,10,15,20-tetrayl]tetrakis-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A



PAGE 2-A

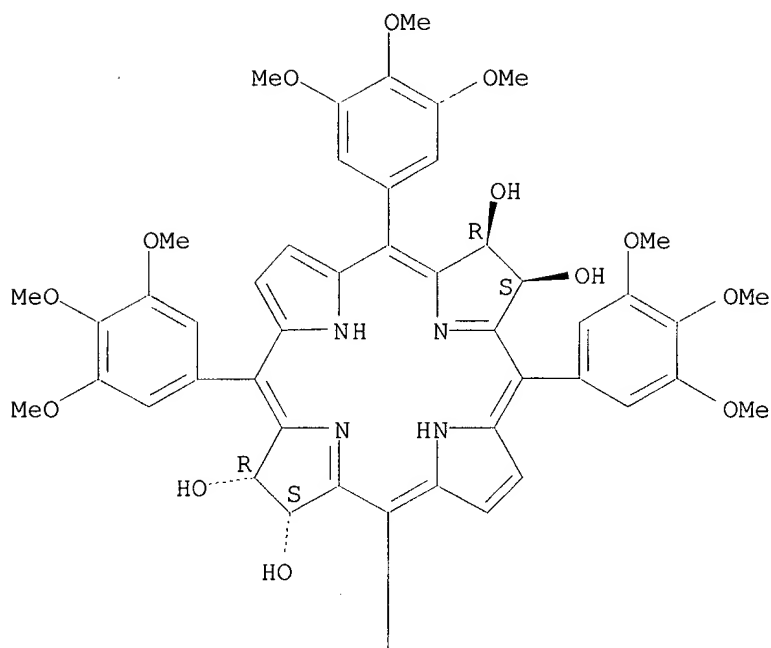


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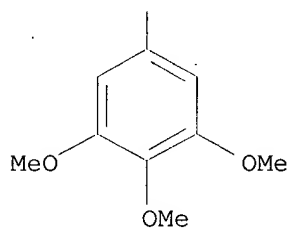
CN 21H,23H-Porphine-7,8,17,18-tetrol, 7,8,17,18-tetrahydro-5,10,15,20-tetrakis(3,4,5-trimethoxyphenyl)-, (7R,8S,17S,18R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

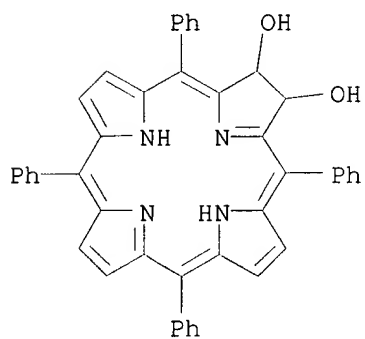
PAGE 1-A



PAGE 2-A

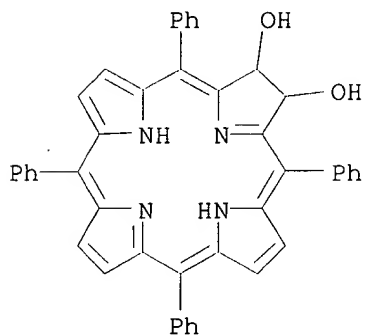


RN 301530-01-8 HCAPLUS  
 CN 21H,23H-Porphine-7,8-diol, 5(or 15)-(4-bromophenyl)-7,8-dihydro-  
 10,15,20(or 5,10,20)-triphenyl-, (7R,8R)-rel- (9CI) (CA INDEX NAME)



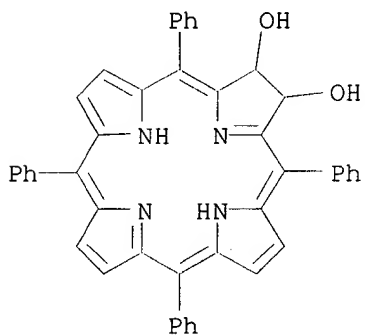
D1- Br

RN 301530-02-9 HCAPLUS  
 CN 21H,23H-Porphine-7,8-diol, 7,8-dihydro-5(or 15)-(4-hydroxyphenyl)-  
 10,15,20(or 5,10,20)-triphenyl-, (7R,8R)-rel- (9CI) (CA INDEX NAME)



D1-OH

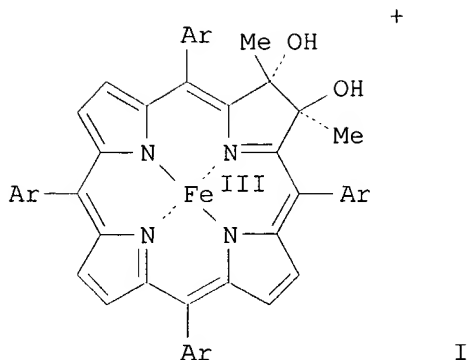
RN 301530-03-0 HCAPLUS  
 CN 21H,23H-Porphine-7,8-diol, 7,8-dihydro-5(or 15)-(4-nitrophenyl)-  
 10,15,20(or 5,10,20)-triphenyl-, (7R,8R)-rel- (9CI) (CA INDEX NAME)

D1-NO<sub>2</sub>

L57 ANSWER 5 OF 8 HCAPLUS COPYRIGHT 2002 ACS  
 AN 1995:751119 HCAPLUS  
 DN 123:216794  
 TI Compound I and II Analogs of a Chlorin  
 AU Jayaraj, K.; Gold, A.; Austin, R. N.; Mandon, D.; Weiss, R.; Turner, J.;  
 Bill, E.; Muether, M.; Trautwein, A. X.  
 CS Department of Environmental Sciences and Engineering, University of North  
 Carolina, Chapel Hill, NC, 27599, USA  
 SO Journal of the American Chemical Society (1995), 117(35),  
 9079-80  
 CODEN: JACSAT; ISSN: 0002-7863  
 PB American Chemical Society  
 DT Journal  
 LA English  
 CC 78-7 (Inorganic Chemicals and Reactions)  
 Section cross-reference(s): 7, 26, 72



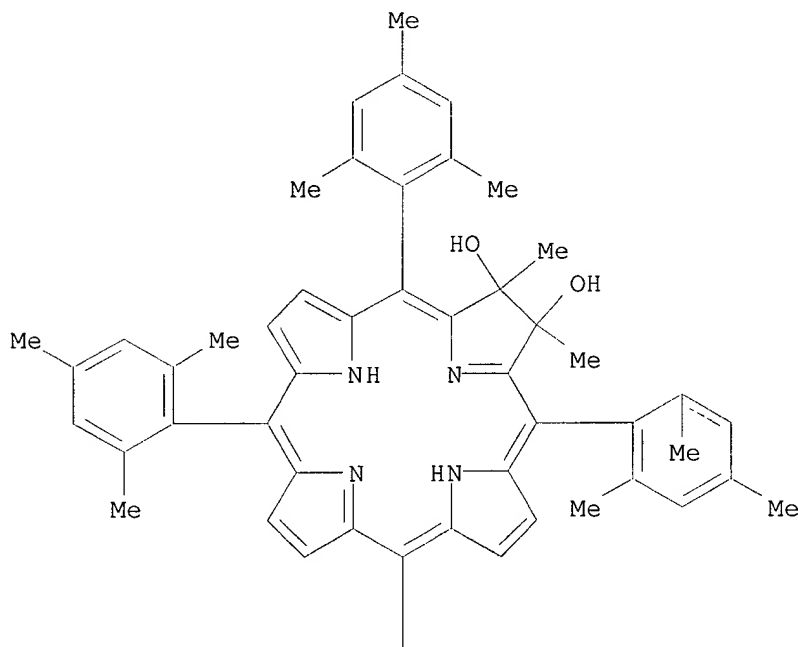
GI



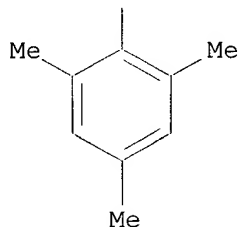
- AB I (Ar = 2,4,6-trimethylphenyl) with coordinated chloride, hydroxide and triflate, were prepd. The 1st electrochem. oxidn. of both the ligand (LH2) and I(Cl) are reversible and are ligand-centered. Oxidn. of I(OH) by m-chloroperbenzoic acid gave [FeIVOL]<sup>+</sup>, a model of the compd. I analog of chlorin, transients of catalases and [FeIVOL], a model of the compd. II analog of chlorin. [FeIVOL]<sup>+</sup> decays to [FeIVOL]. The complexes were characterized by various techniques such as EPR, Moessbauer, UV-visible and resonance Raman spectroscopy.
- ST chlorin compd I II analog; catalase transient model iron 4 complex; ferryl chlorin pi cation radical; electrochem chlorin iron complex
- IT Enzyme functional sites  
RL: BSU (Biological study, unclassified); BIOL (Biological study) (ferryl chlorin complexes as models of compd. I and II analogs of catalase)
- IT Oxidation, electrochemical  
(of chlorin deriv. and metal-free base)
- IT 167774-53-0 **167936-43-8**  
RL: FMU (Formation, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); FORM (Formation, nonpreparative); PROC (Process); RACT (Reactant or reagent) (electrochem. formation and elec. potential of couple contg.)
- IT 9001-05-2, Catalase  
RL: BSU (Biological study, unclassified); BIOL (Biological study) (ferryl chlorin complexes as models of compd. I and II analogs of)
- IT 167774-52-9P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (prepn. and metatheses)
- IT 167774-54-1P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (prepn. and oxidn.)
- IT **167774-51-8P**  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (prepn. and reaction with ferrous chloride)
- IT 167774-56-3P  
RL: BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent) (prepn. as compd. I analog of chlorin and decay to compd. II analog)
- IT 167774-57-4P  
RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(prepn. as compd. II analog of chlorin)  
 IT 167774-55-2P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. of)  
 IT 167774-58-5, 2,3-Dioxo-meso-tetramesitylporphyrin  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction with methyllithium)  
 IT 167936-43-8  
 RL: FMU (Formation, unclassified); PEP (Physical, engineering or chemical  
 process); PRP (Properties); RCT (Reactant); FORM (Formation,  
 nonpreparative); PROC (Process); RACT (Reactant or reagent)  
 (electrochem. formation and elec. potential of couple contg.)  
 RN 167936-43-8 HCAPLUS  
 CN 21H,23H-Porphine-7,8-diol, 7,8-dihydro-7,8-dimethyl-5,10,15,20-  
 tetrakis(2,4,6-trimethylphenyl)-, radical ion(1+), (7R,8R)-rel- (9CI) (CA  
 INDEX NAME)

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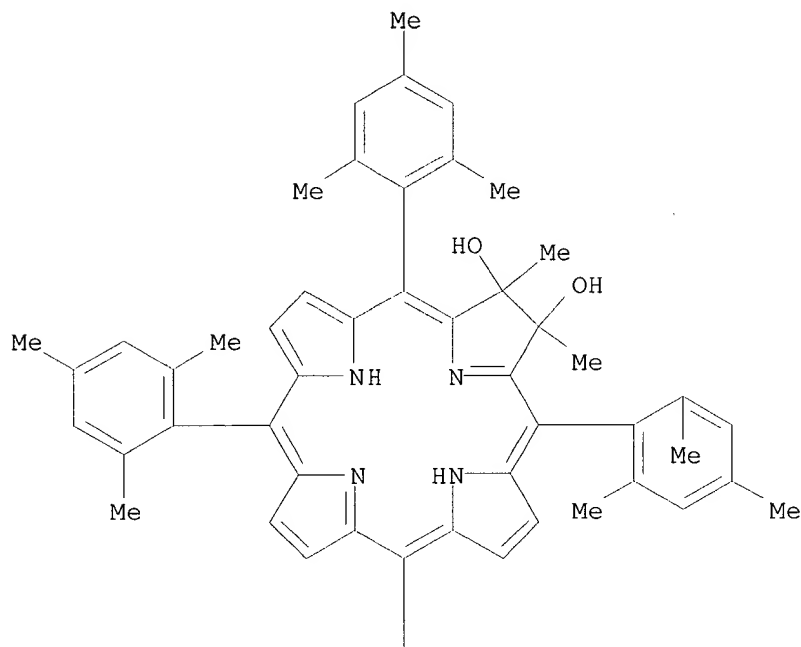
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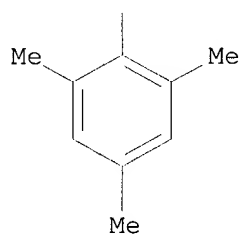
IT 167774-51-8P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (prepn. and reaction with ferrous chloride)

RN 167774-51-8 HCAPLUS  
 CN 21H,23H-Porphine-7,8-diol, 7,8-dihydro-7,8-dimethyl-5,10,15,20-tetrakis(2,4,6-trimethylphenyl)-, (7R,8R)-rel- (9CI) (CA INDEX NAME)

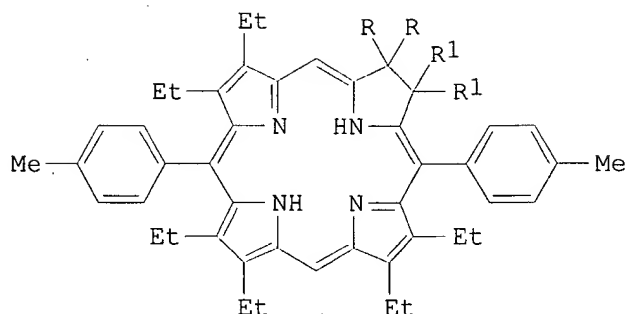
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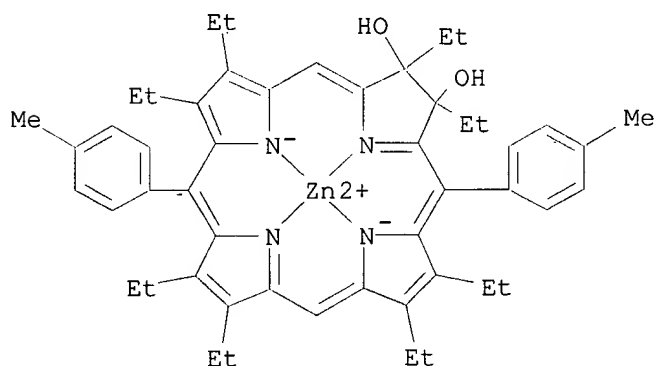


L57 ANSWER 6 OF 8 HCAPLUS COPYRIGHT 2002 ACS  
 AN 1994:408966 HCAPLUS  
 DN 121:8966  
 TI Synthesis of 5,15-diaryl-substituted oxochlorins from 5,15-diaryloctaethylporphyrin  
 AU Osuka, Atsuhiko; Marumo, Shinji; Maruyama, Kazuhiro  
 CS Fac. Sci., Kyoto Univ., Kyoto, 606, Japan  
 SO Bulletin of the Chemical Society of Japan (1993), 66(12), 3837-9  
 CODEN: BCSJA8; ISSN: 0009-2673  
 DT Journal  
 LA English  
 CC 26-7 (Biomolecules and Their Synthetic Analogs)  
 Section cross-reference(s): 11  
 GI



I

- AB 5,15-Diaryl-substituted oxochlorins I (R = Et, R12 = O; R2 = O, R1 = Et) were prepd. from osmium tetroxide oxidn. of 5,15-diaryloctaethylporphyrin followed by acid-catalyzed pinacol rearrangement. Optical and electrochem. properties of this macrocyclic ring are studied by measuring the absorption and fluorescence spectra, fluorescence lifetimes, and one-electron oxidn. and redn. potentials.
- ST oxochlorin diaryl photosynthetic reaction center model; diaryloctaethylporphyrin
- IT Photosynthetic systems  
(reaction center, prepn. of diaryl oxochlorins toward construction of a model)
- IT 65858-48-2 155737-00-1  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(oxidn. with osmium tetroxide)
- IT **155737-01-2P**  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. and rearrangement)
- IT 155527-06-3P 155527-07-4P 155737-02-3P 155760-99-9P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of)
- IT **155737-01-2P**  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. and rearrangement)
- RN 155737-01-2 HCAPLUS
- CN Zinc, [rel-(7R,8S)-2,3,7,8,12,13,17,18-octaethyl-7,8-dihydro-5,15-bis(4-methylphenyl)-21H,23H-porphine-7,8-diolato(2-)-.kappa.N21,.kappa.N22,.kappa.N23,.kappa.N24]-, (SP-4-2)- (9CI) (CA INDEX NAME)



AN 1991:418425 HCAPLUS  
DN 115:18425  
TI Photochemistry and radiation chemistry of the .beta.-cyclodextrin-ZnTSPP inclusion complex  
AU Mosseri, S.; Mialocq, J. C.  
CS CEA, CEN Saclay, Gif-sur-Yvette, F-91191, Fr.  
SO Radiation Physics and Chemistry (1991), 37(5-6), 653-6  
CODEN: RPCHDM; ISSN: 0146-5724  
DT Journal  
LA English  
CC 74-1 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)  
AB Steady-state and pulse radiolysis combined with optical and conductimetric anal. and steady-state photolysis were used to characterize the intermediates and the stable products formed upon oxidn. of zinc tetrakis(4-sulfonatophenyl)porphyrin (ZnTSPP) in aq. soln. in the presence and absence of .beta.-cyclodextrin (.beta.-CD). In the absence of .beta.-CD, its oxidn. either by the OH.bul., primary species of the radiolysis of water, or photooxidn. by O2 lead to mixts. of products (partially unidentified) which reflect the poor selectivity of the oxidizing species. In the presence of .beta.-CD, a highly selective formation (99%) of the porphyrin dication is obsd. upon 422 nm photolysis of an aerated soln. of ZnTSPP at pH = 12. The dramatic effect of the porphyrin complexation by .beta.-CD is emphasized.  
ST photolysis zinc porphyrin cyclodextrin inclusion complex; radiolysis zinc porphyrin cyclodextrin inclusion complexes; photooxidn zinc porphyrin cyclodextrin inclusion complex  
IT Electron exchange  
(in photooxidn. of zinc tetrakis(sulfonatophenyl)porphyrin in presence of cyclodextrin, reaction products in)  
IT Fluorescence  
(of photooxidn. products of zinc tetrakis(sulfonatophenyl)porphyrin, effect of cyclodextrin inclusion complex formation on)  
IT Ultraviolet and visible spectra  
(of photoproduct in photooxidn. of zinc tetrakis(sulfonatophenyl)porphyrin, effect of cyclodextrin inclusion complex formation on)  
IT Radiolysis  
(of zinc tetrakis(sulfonatophenyl)porphyrin in presence and absence of cyclodextrin)  
IT Oxidation, photochemical  
(of zinc tetrakis(sulfonatophenyl)porphyrin in presence and absence of cyclodextrin, reaction products in)  
IT Photolysis  
(of zinc tetrakis(sulfonatophenyl)porphyrin, in presence and absence of cyclodextrin, oxidn. products in)  
IT 133551-73-2P  
RL: FORM (Formation, nonpreparative); PREP (Preparation)  
(formation of, in photooxidn. of zinc tetrakis(sulfonatophenyl)porphyrin, reaction intermediates and products studied by pulse radiolysis and steady state photolysis)  
IT 7585-39-9, .beta.-Cyclodextrin  
RL: USES (Uses)  
(photooxidn. of zinc tetrakis(sulfonatophenyl)porphyrin in presence and absence of, reaction intermediates and products in)  
IT 56047-87-1  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(photooxidn. of, in presence and absence of cyclodextrin, reaction intermediates and products in, radiolysis and photolysis study of)  
IT 3352-57-6, Hydroxyl radical, reactions  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, in radiolysis of zinc tetrakis(sulfonatophenyl)porphyrin in aq. soln. in presence and absence of .beta.-cyclodextrin, photooxidn. products in)

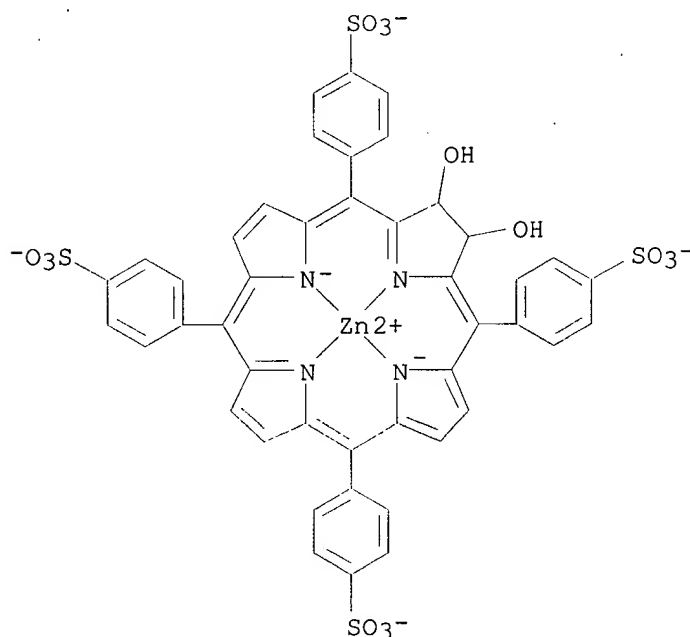
IT 7782-44-7, Oxygen, reactions  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with triplet excited state of zinc  
 tetrakis(sulfonatophenyl)porphyrin in .beta.-cyclodextrin inclusion  
 complex, photooxidn. products in)

IT 133551-73-2P  
 RL: FORM (Formation, nonpreparative); PREP (Preparation)  
 (formation of, in photooxidn. of zinc tetrakis(sulfonatophenyl)porphyrin,  
 reaction intermediates and products studied by pulse radiolysis and  
 steady state photolysis)

RN 133551-73-2 HCAPLUS

CN Zincate(4-), [[4,4',4'',4'''-(7,8-dihydro-7,8-dihydroxy-21H,23H-porphine-5,10,15,20-tetrayl-.kappa.N21,.kappa.N22,.kappa.N23,.kappa.N24)tetrakis(benzenesulfonato)](6-)]-, tetrahydrogen, (SP-4-1)- (9CI) (CA INDEX NAME)

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● 4 H<sup>+</sup>

L57 ANSWER 8 OF 8 HCAPLUS COPYRIGHT 2002 ACS

AN 1991:217823 HCAPLUS

DN 114:217823

TI Porphyrins-cyclodextrin. 1. Photooxidation of zinc tetrakis(4-sulfonatophenyl)porphyrin (ZnTSP) in cyclodextrin cavities: the characterization of ZnTSP dication. Photolysis, radiolysis, and NMR studies

AU Mosseri, S.; Mialocq, J. C.; Perly, B.; Hambright, P.

CS DPhG, CEA-CEN Saclay, Gif-sur-Yvette, F-91191, Fr.

SO Journal of Physical Chemistry (1991), 95(6), 2196-203

CODEN: JPCHAX; ISSN: 0022-3654

DT Journal

- LA English
- CC 74-1 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)
- AB NMR and spectrophotometric evidence for the formation of a 4:1 cyclodextrin-zinc tetrakis(4-sulfonatophenyl)porphyrin (ZnTSPP) (CD-ZnP) complex is reported. Photolysis of CD-ZnP at 422 nm at pH = 12 led to quant. formation (99.9%) of 1,2-dihydroxyporphyrin, with intense absorption bands at 340 and 625 nm and an emission band at 642 nm. At much lower pH the photolysis led to the efficient formation of isoporphyrin or its hydroxylated form ( $pK = 6.0$ ), with characteristic absorption bands in the .apprx.IR region. The nonfluorescing isoporphyrin was converted slowly via mol. rearrangement and further hydroxylation into the fluorescing 1,2-dihydroxyporphyrin ( $k = 1.1 \text{ M}^{-1} \text{ s}^{-1}$ ). Emission and excitation spectra of the final stable products are reported. OH.bul. radical also led to the formation (although inefficient) of 1,2-dihydroxyporphyrin as shown by .gamma.-radiolysis and pulse radiolysis expts. Pulse radiolysis expts. in the presence of  $\text{Br}^-$  were carried out as well. Inhibition of the electron transfer from ZnTSPP to the  $\text{Br}_2$ .bul.-radical in cyclodextrin soln. was obsd. and investigated in detail. The photophys. properties of the inclusion complex and of  $\text{ZnTSPP}^{2+}$  were detd. by using the time-correlated single-photon-counting technique and the nanosecond laser absorption spectroscopy method. The absorption spectra of  $\text{ZnTSPP}$ .bul. $^{3+}$  and  $\text{ZnTSPP}^{4+}$  are also reported.
- ST zinc porphyrin photooxidn cyclodextrin cavity; photolysis zinc porphyrin cyclodextrin; radiolysis zinc porphyrin cyclodextrin; photophys zinc porphyrin cyclodextrin inclusion complex
- IT Ultraviolet and visible spectra  
(of zinc tetrakis(sulfonatophenyl)porphyrin hydroxylated dication and trication radical and tetracation, photoresistant radiolysis in study of)
- IT Oxidation, photochemical  
(of zinc tetrakis(sulfonatophenyl)porphyrin in cyclodextrin cavities, characterization of dication produced in)
- IT Photolysis  
(of zinc tetrakis(sulfonatophenyl)porphyrin in cyclodextrin cavities, characterization of porphyrin dication produced in)
- IT Nuclear magnetic resonance  
(of zinc tetrakis(sulfonatophenyl)porphyrin-cyclodextrin inclusion compds., photochem. and photophysics in relation to)
- IT Radiolysis  
(pulsed, of zinc tetrakis(sulfonatophenyl)porphyrin solns. in presence of cyclodextrin)
- IT 133551-74-3P 133578-09-3P  
RL: PRP (Properties); PREP (Preparation)  
(formation and optical absorption spectrum of, in photooxidn. of zinc tetrakis(sulfonatophenyl)porphyrin in cyclodextrin cavities)
- IT 133551-73-2P 133578-24-2P  
RL: FORM (Formation, nonpreparative); PREP (Preparation)  
(formation of, in photolysis of zinc tetrakis(sulfonatophenyl)porphyrin in cyclodextrin cavities)
- IT 133551-72-1P  
RL: FORM (Formation, nonpreparative); PREP (Preparation)  
(formation of, in photooxidn. of zinc tetrakis(sulfonatophenyl)porphyrin in cyclodextrin cavities)
- IT 79346-67-1P  
RL: FORM (Formation, nonpreparative); PREP (Preparation)  
(formation of, in radiolysis of zinc tetrakis(sulfonatophenyl)porphyrin in aq. soln. contg. cyclodextrin)
- IT 7585-39-9, .beta.-Cyclodextrin  
RL: USES (Uses)  
(photooxidn. of zinc tetrakis(sulfonatophenyl)porphyrin in cavities of, characterization of porphyrin dication produced in, radiolysis and NMR studies in)

IT 56047-87-1  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (photooxidn. of, in cyclodextrin cavities, radiolysis and NMR studies  
 in characterization of dication produced in)

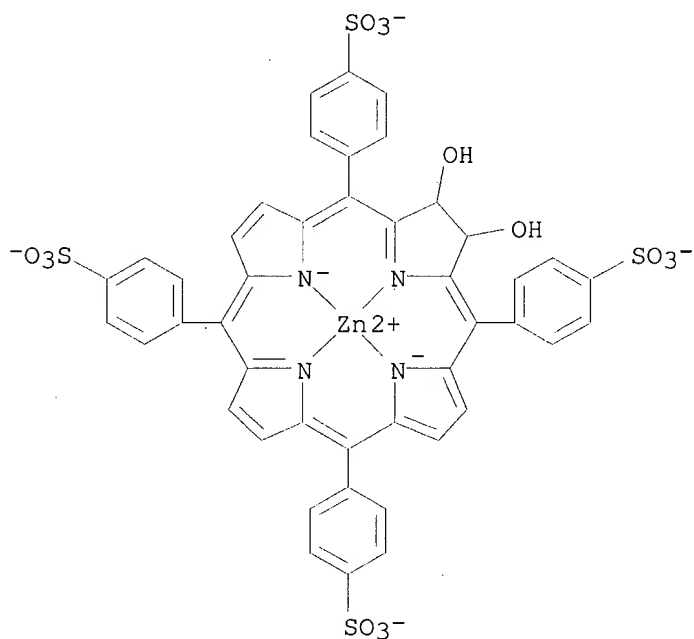
IT 24959-67-9, Bromide, uses and miscellaneous  
 RL: USES (Uses)  
 (radiolysis of zinc tetrakis(sulfonatophenyl)porphyrin in presence of,  
 cyclodextrin effect on inhibition of electron transfer in)

IT 133551-73-2P  
 RL: FORM (Formation, nonpreparative); PREP (Preparation)  
 (formation of, in photolysis of zinc tetrakis(sulfonatophenyl)porphyrin  
 in cyclodextrin cavities)

RN 133551-73-2 HCAPLUS

CN Zincate(4-), [[4,4',4'',4'''-(7,8-dihydro-7,8-dihydroxy-21H,23H-porphine-  
 5,10,15,20-tetrayl-.kappa.N21,.kappa.N22,.kappa.N23,.kappa.N24)tetrakis[be  
 nzenesulfonato]](6-)]-, tetrahydrogen, (SP-4-1)- (9CI) (CA INDEX NAME)

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● 4 H<sup>+</sup>

=&gt; fil reg

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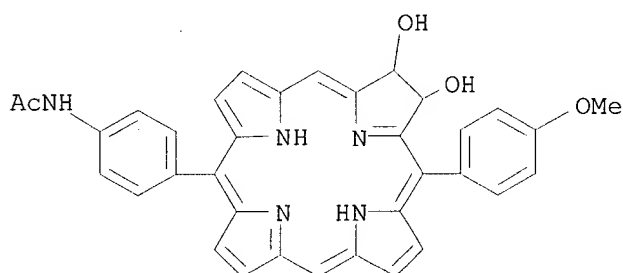
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conducting SmartSELECT searches.

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PROPERTIES for more information. See STNote 27, Searching Properties  
in the CAS Registry File, for complete details:  
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

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L49 ANSWER 1 OF 35 REGISTRY COPYRIGHT 2002 ACS  
RN 414866-61-8 REGISTRY  
CN **Acetamide, N-[4-[17,18-dihydro-17,18-dihydroxy-15-(4-methoxyphenyl)-  
21H,23H-porphin-5-yl]phenyl]- (9CI) (CA INDEX NAME)**  
MF C35 H29 N5 O4  
SR CA  
LC STN Files: CA, CAPLUS



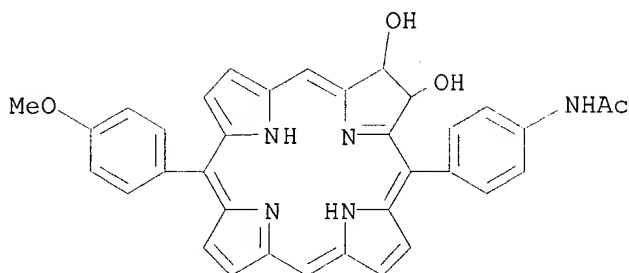
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1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 136:321357

L49 ANSWER 2 OF 35 REGISTRY COPYRIGHT 2002 ACS  
RN 414866-60-7 REGISTRY  
CN **Acetamide, N-[4-[7,8-dihydro-7,8-dihydroxy-15-(4-methoxyphenyl)-  
21H,23H-porphin-5-yl]phenyl]- (9CI) (CA INDEX NAME)**  
MF C35 H29 N5 O4  
SR CA  
LC STN Files: CA, CAPLUS



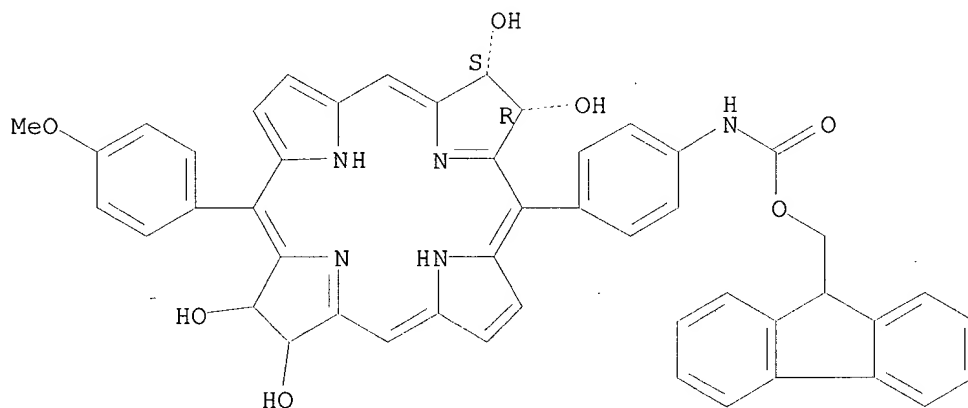
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1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 136:321357

L49 ANSWER 3 OF 35 REGISTRY COPYRIGHT 2002 ACS  
RN 414866-59-4 REGISTRY  
CN Carbamic acid, [4-[(7R,8S)-7,8,17,18-tetrahydro-7,8,17,18-tetrahydroxy-15-(4-methoxyphenyl)-21H,23H-porphin-5-yl]phenyl]-, 9H-fluoren-9-ylmethyl ester, rel- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C48 H39 N5 O7  
SR CA  
LC STN Files: CA, CAPLUS

Relative stereochemistry.



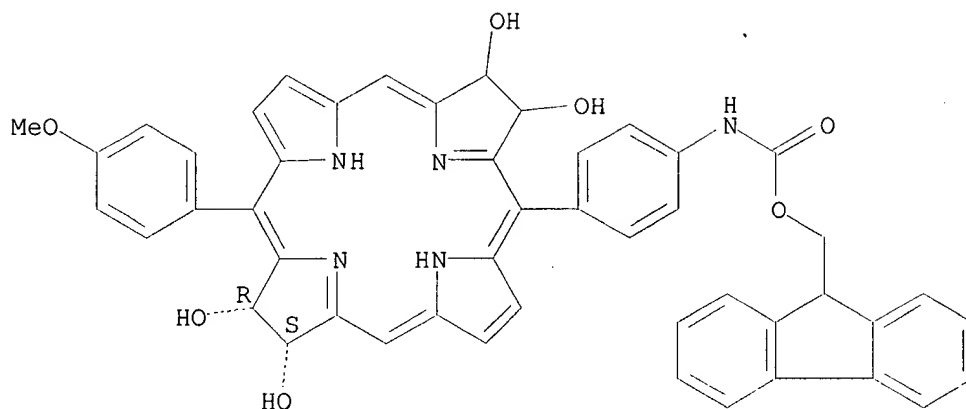
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1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 136:321357

L49 ANSWER 4 OF 35 REGISTRY COPYRIGHT 2002 ACS  
RN 414866-58-3 REGISTRY  
CN Carbamic acid, [4-[(17R,18S)-7,8,17,18-tetrahydro-7,8,17,18-tetrahydroxy-15-(4-methoxyphenyl)-21H,23H-porphin-5-yl]phenyl]-, 9H-fluoren-9-ylmethyl ester, rel- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C48 H39 N5 O7  
SR CA

LC STN Files: CA, CAPLUS

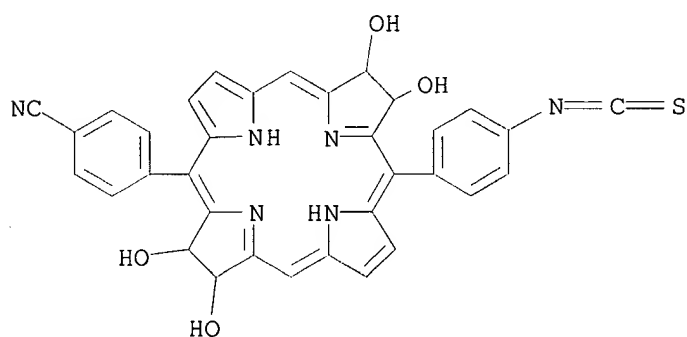
Relative stereochemistry.



1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 136:321357

L49 ANSWER 5 OF 35 REGISTRY COPYRIGHT 2002 ACS  
RN 385384-86-1 REGISTRY  
CN **Benzonitrile, 4-[7,8,17,18-tetrahydro-7,8,17,18-tetrahydroxy-15-(4-isothiocyanatophenyl)-21H,23H-porphin-5-yl]- (9CI)** (CA INDEX NAME)  
MF C34 H24 N6 O4 S  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER



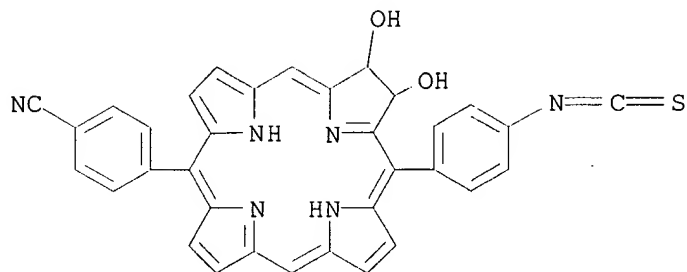
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1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 136:69694

L49 ANSWER 6 OF 35 REGISTRY COPYRIGHT 2002 ACS  
RN 385384-85-0 REGISTRY  
CN **Benzonitrile, 4-[17,18-dihydro-17,18-dihydroxy-15-(4-isothiocyanatophenyl)-21H,23H-porphin-5-yl]- (9CI)** (CA INDEX NAME)  
MF C34 H22 N6 O2 S  
SR CA

LC STN Files: CA, CAPLUS, TOXCENTER

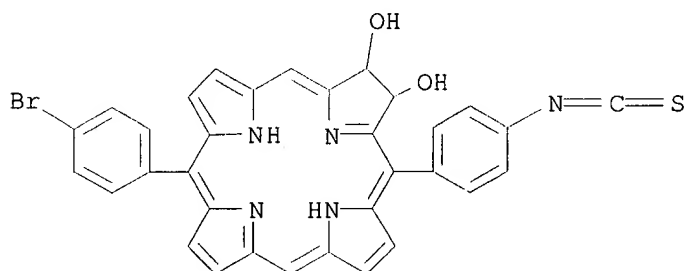


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1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 136:69694

L49 ANSWER 7 OF 35 REGISTRY COPYRIGHT 2002 ACS  
RN 385384-84-9 REGISTRY  
CN **21H,23H-Porphine-7,8-diol, 15-(4-bromophenyl)-7,8-dihydro-5-(4-isothiocyanatophenyl)-(9CI)** (CA INDEX NAME)  
MF C33 H22 Br N5 O2 S  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER

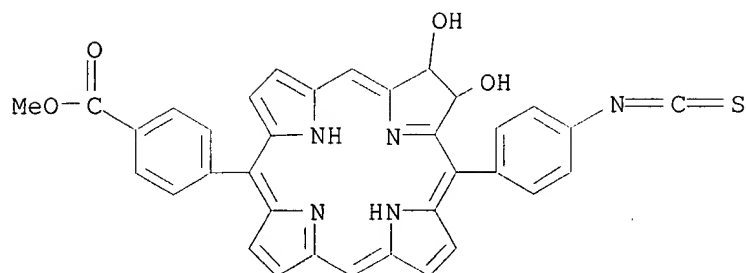


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 136:69694

L49 ANSWER 8 OF 35 REGISTRY COPYRIGHT 2002 ACS  
RN 385384-83-8 REGISTRY  
CN **Benzoic acid, 4-[17,18-dihydro-17,18-dihydroxy-15-(4-isothiocyanatophenyl)-21H,23H-porphin-5-yl]-, methyl ester (9CI)** (CA INDEX NAME)  
MF C35 H25 N5 O4 S  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER

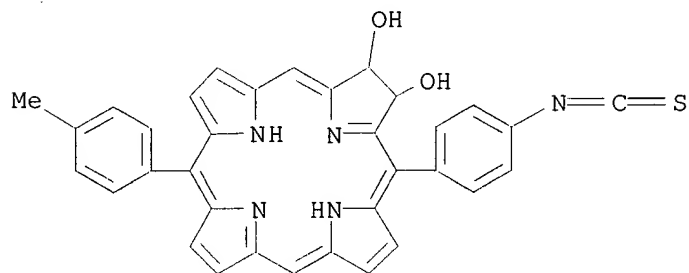


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 136:69694

L49 ANSWER 9 OF 35 REGISTRY COPYRIGHT 2002 ACS  
RN 385384-79-2 REGISTRY  
CN **21H,23H-Porphine-7,8-diol, 7,8-dihydro-5-(4-isothiocyanatophenyl)-15-(4-methylphenyl)- (9CI)** (CA INDEX NAME)  
MF C34 H25 N5 O2 S  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER

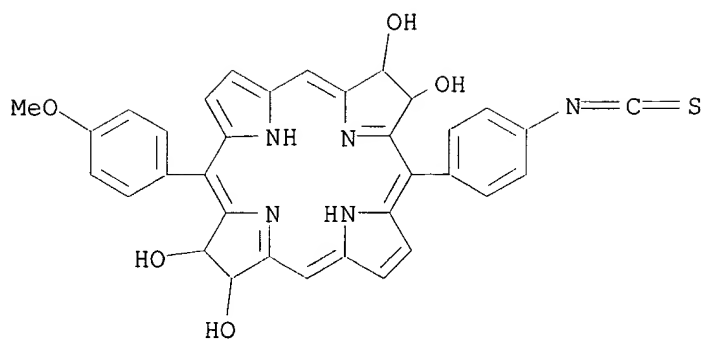


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 136:69694

L49 ANSWER 10 OF 35 REGISTRY COPYRIGHT 2002 ACS  
RN 385384-77-0 REGISTRY  
CN **21H,23H-Porphine-7,8,17,18-tetrol, 7,8,17,18-tetrahydro-5-(4-isothiocyanatophenyl)-15-(4-methoxyphenyl)- (9CI)** (CA INDEX NAME)  
MF C34 H27 N5 O5 S  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER

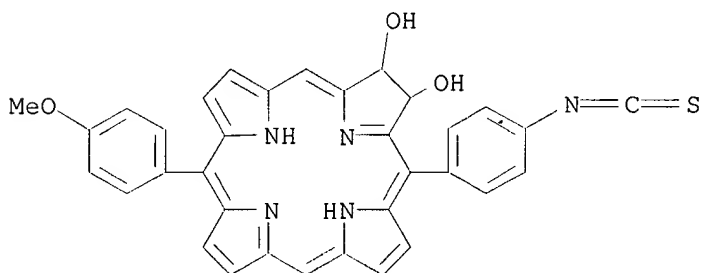


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 136:69694

L49 ANSWER 11 OF 35 REGISTRY COPYRIGHT 2002 ACS  
RN 385384-76-9 REGISTRY  
CN **21H,23H-Porphine-7,8-diol, 7,8-dihydro-5-(4-isothiocyanatophenyl)-15-(4-methoxyphenyl)- (9CI)** (CA INDEX NAME)  
MF C34 H25 N5 O3 S  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER

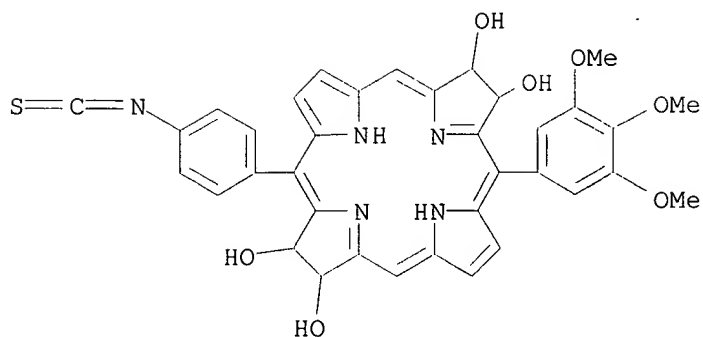


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 136:69694

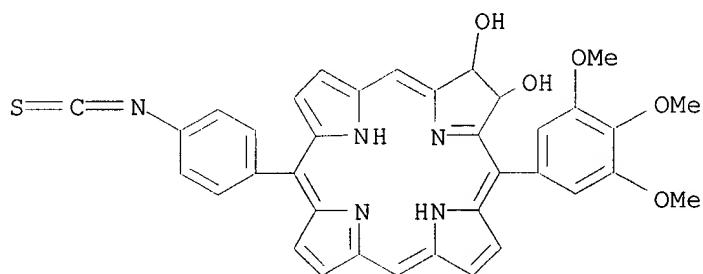
L49 ANSWER 12 OF 35 REGISTRY COPYRIGHT 2002 ACS  
RN 385384-74-7 REGISTRY  
CN **21H,23H-Porphine-7,8,17,18-tetrol, 7,8,17,18-tetrahydro-5-(4-isothiocyanatophenyl)-15-(3,4,5-trimethoxyphenyl)- (9CI)** (CA INDEX NAME)  
MF C36 H31 N5 O7 S  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER



1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 136:69694

L49 ANSWER 13 OF 35 REGISTRY COPYRIGHT 2002 ACS  
RN 385384-73-6 REGISTRY  
CN **21H,23H-Porphine-7,8-diol, 7,8-dihydro-15-(4-isothiocyanatophenyl)-5-(3,4,5-trimethoxyphenyl)-(9CI)** (CA INDEX NAME)  
MF C36 H29 N5 O5 S  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER

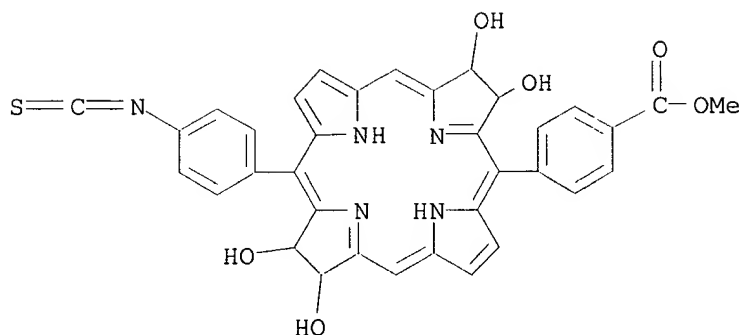


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

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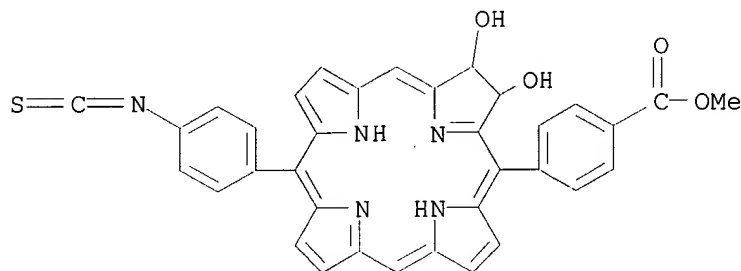
L49 ANSWER 14 OF 35 REGISTRY COPYRIGHT 2002 ACS  
RN 385384-71-4 REGISTRY  
CN **Benzoic acid, 4-[7,8,17,18-tetrahydro-7,8,17,18-tetrahydroxy-15-(4-isothiocyanatophenyl)-21H,23H-porphin-5-yl]-, methyl ester (9CI)** (CA INDEX NAME)  
MF C35 H27 N5 O6 S  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER



1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 136:69694

L49 ANSWER 15 OF 35 REGISTRY COPYRIGHT 2002 ACS  
RN 385384-70-3 REGISTRY  
CN **Benzoic acid, 4-[7,8-dihydro-7,8-dihydroxy-15-(4-isothiocyanatophenyl)-21H,23H-porphin-5-yl]-, methyl ester (9CI)** (CA INDEX NAME)  
MF C35 H25 N5 O4 S  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER



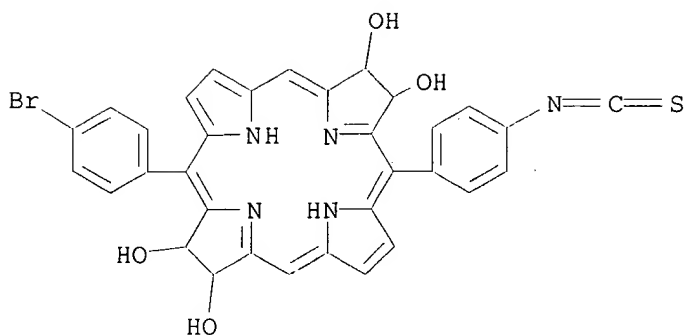
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1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 136:69694

L49 ANSWER 16 OF 35 REGISTRY COPYRIGHT 2002 ACS  
RN 385384-68-9 REGISTRY  
CN **21H,23H-Porphine-7,8,17,18-tetrol, 5-(4-bromophenyl)-7,8,17,18-tetrahydro-15-(4-isothiocyanatophenyl)- (9CI)** (CA INDEX NAME)  
MF C33 H24 Br N5 O4 S  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER



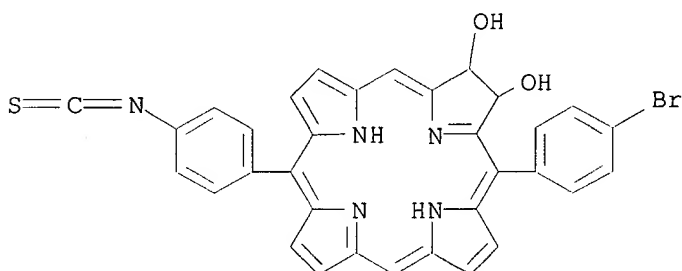


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 136:69694

L49 ANSWER 17 OF 35 REGISTRY COPYRIGHT 2002 ACS  
RN 385384-67-8 REGISTRY  
CN 21H,23H-Porphine-7,8-diol, 5-(4-bromophenyl)-7,8-dihydro-15-(4-isothiocyanatophenyl)- (9CI) (CA INDEX NAME)  
MF C33 H22 Br N5 O2 S  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER

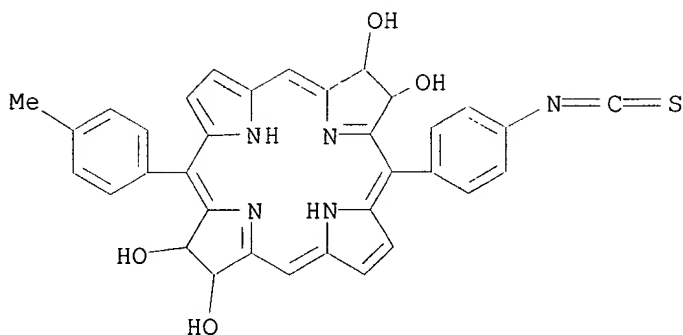


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 136:69694

L49 ANSWER 18 OF 35 REGISTRY COPYRIGHT 2002 ACS  
RN 385384-65-6 REGISTRY  
CN 21H,23H-Porphine-7,8,17,18-tetrol, 7,8,17,18-tetrahydro-5-(4-isothiocyanatophenyl)-15-(4-methylphenyl)- (9CI) (CA INDEX NAME)  
MF C34 H27 N5 O4 S  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER

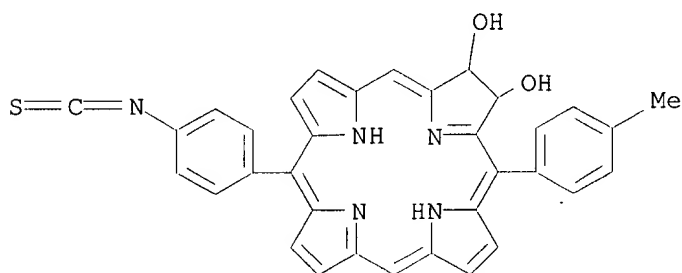


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1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 136:69694

L49 ANSWER 19 OF 35 REGISTRY COPYRIGHT 2002 ACS  
RN 385384-64-5 REGISTRY  
CN **21H,23H-Porphine-7,8-diol, 7,8-dihydro-15-(4-isothiocyanatophenyl)-5-(4-methylphenyl)- (9CI)** (CA INDEX NAME)  
MF C34 H25 N5 O2 S  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER



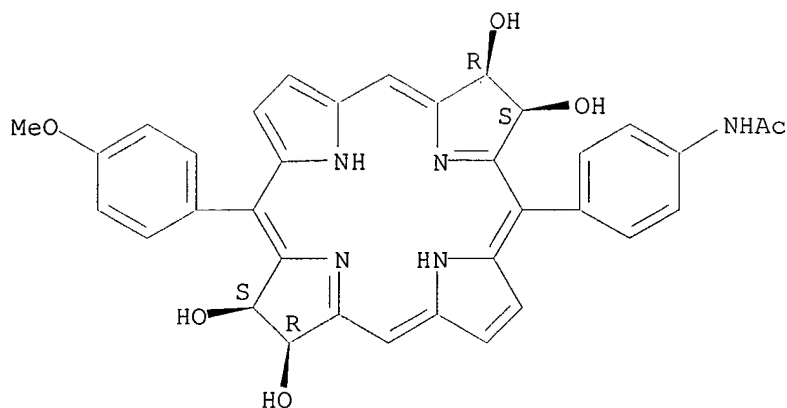
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 136:69694

L49 ANSWER 20 OF 35 REGISTRY COPYRIGHT 2002 ACS  
RN 385384-59-8 REGISTRY  
CN **Acetamide, N-[4-[(7R,8S,17R,18S)-7,8,17,18-tetrahydro-7,8,17,18-tetrahydroxy-15-(4-methoxyphenyl)-21H,23H-porphin-5-yl]phenyl]-, rel-(9CI)** (CA INDEX NAME)  
FS STEREOSEARCH  
MF C35 H31 N5 O6  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER

Relative stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

2 REFERENCES IN FILE CA (1962 TO DATE)  
2 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 136:321357

REFERENCE 2: 136:69694

L49 ANSWER 21 OF 35 REGISTRY COPYRIGHT 2002 ACS

RN 385384-58-7 REGISTRY

CN **Acetamide, N-[4-[(7R,8S,17S,18R)-7,8,17,18-tetrahydro-7,8,17,18-tetrahydroxy-15-(4-methoxyphenyl)-21H,23H-porphin-5-yl]phenyl]-, rel-(9CI)** (CA INDEX NAME)

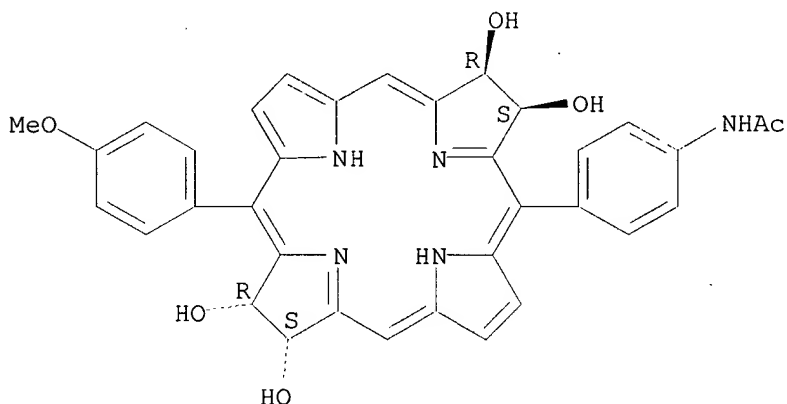
FS STEREOSEARCH

MF C35 H31 N5 O6

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER

Relative stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

2 REFERENCES IN FILE CA (1962 TO DATE)  
2 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 136:321357

REFERENCE 2: 136:69694

L49 ANSWER 22 OF 35 REGISTRY COPYRIGHT 2002 ACS

RN 385384-57-6 REGISTRY

CN **Acetamide, N-[4-[(7R,8S)-7,8-dihydro-7,8-dihydroxy-15-(4-methoxyphenyl)-21H,23H-porphin-5-yl]phenyl]-, rel- (9CI)** (CA INDEX NAME)

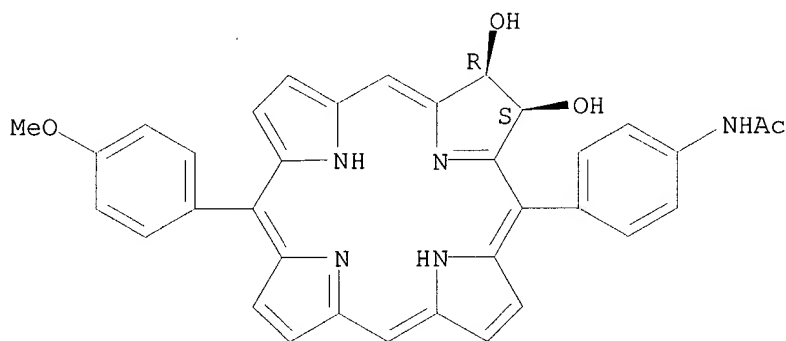
FS STEREOSEARCH

MF C35 H29 N5 O4

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER

Relative stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1962 TO DATE)

1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 136:69694

L49 ANSWER 23 OF 35 REGISTRY COPYRIGHT 2002 ACS

RN 385384-56-5 REGISTRY

CN **Acetamide, N-[4-[(17R,18S)-17,18-dihydro-17,18-dihydroxy-15-(4-methoxyphenyl)-21H,23H-porphin-5-yl]phenyl]-, rel- (9CI)** (CA INDEX NAME)

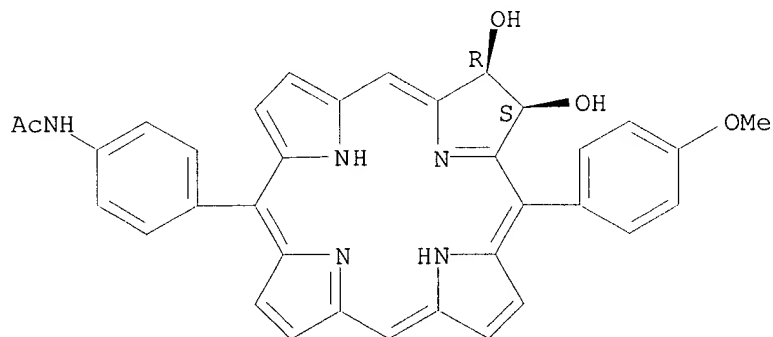
FS STEREOSEARCH

MF C35 H29 N5 O4

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER

Relative stereochemistry.



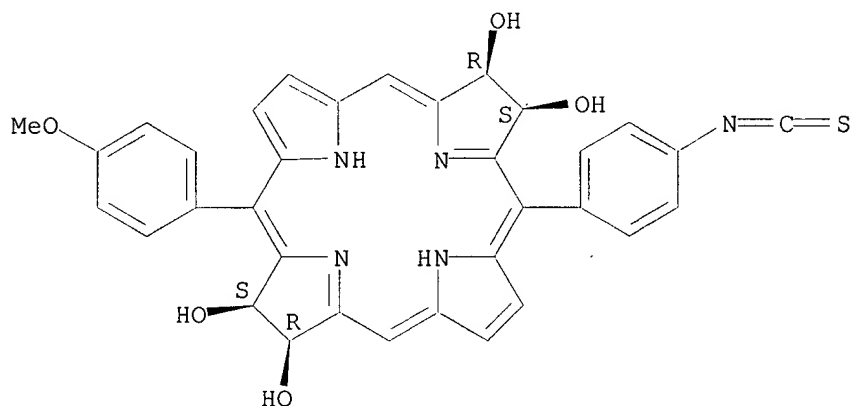
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 136:69694

L49 ANSWER 24 OF 35 REGISTRY COPYRIGHT 2002 ACS  
RN 385384-55-4 REGISTRY  
CN 21H,23H-Porphine-7,8,17,18-tetrol, 7,8,17,18-tetrahydro-5-(4-isothiocyanatophenyl)-15-(4-methoxyphenyl)-, (7R,8S,17R,18S)-rel- (9CI)  
(CA INDEX NAME)  
FS STEREOSEARCH  
MF C34 H27 N5 O5 S  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER

Relative stereochemistry.



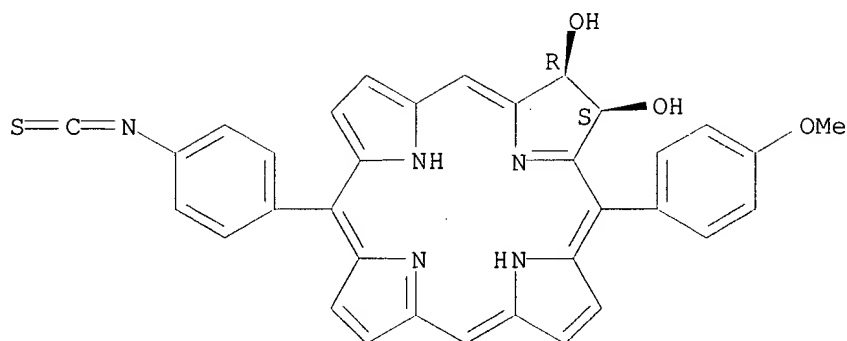
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1962 TO DATE)  
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REFERENCE 1: 136:69694

L49 ANSWER 25 OF 35 REGISTRY COPYRIGHT 2002 ACS  
RN 385384-54-3 REGISTRY  
CN 21H,23H-Porphine-7,8-diol, 7,8-dihydro-15-(4-isothiocyanatophenyl)-5-(4-methoxyphenyl)-, (7R,8S)-rel- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C34 H25 N5 O3 S  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER

Relative stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

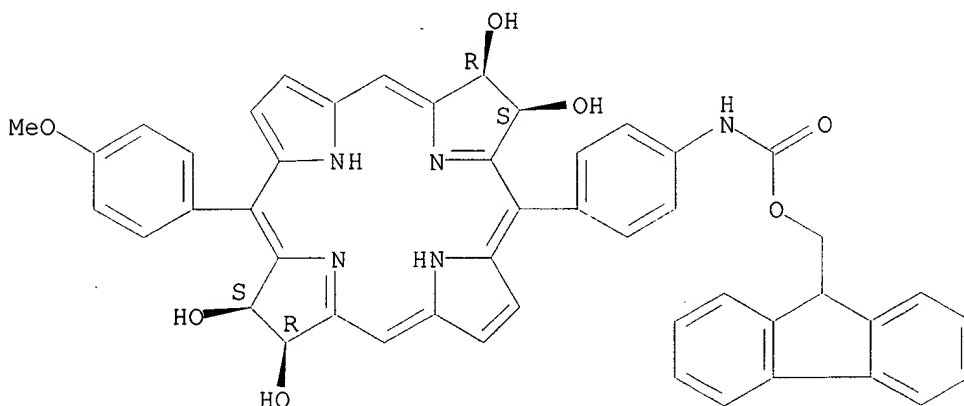
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REFERENCE 1: 136:321357

REFERENCE 2: 136:69694

L49 ANSWER 26 OF 35 REGISTRY COPYRIGHT 2002 ACS  
RN 385384-46-3 REGISTRY  
CN Carbamic acid, [4-[(7R,8S,17R,18S)-7,8,17,18-tetrahydro-7,8,17,18-tetrahydroxy-15-(4-methoxyphenyl)-21H,23H-porphin-5-yl]phenyl]-, 9H-fluoren-9-ylmethyl ester, rel- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C48 H39 N5 O7  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER

Relative stereochemistry.



1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

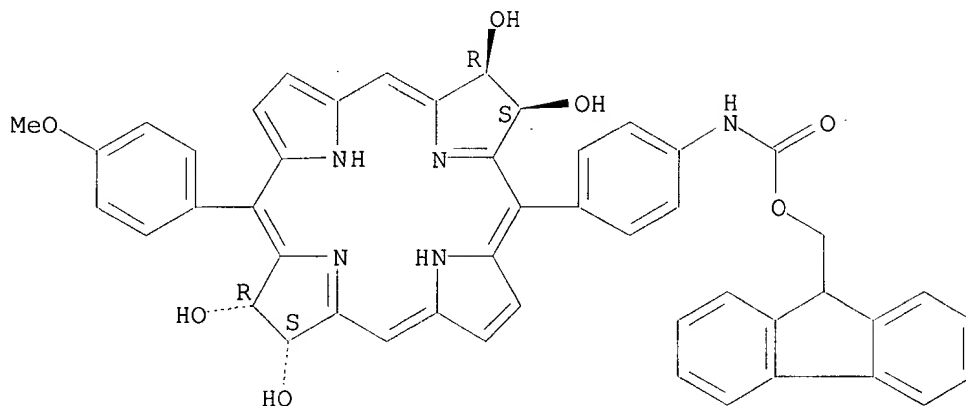
REFERENCE 1: 136:69694

L49 ANSWER 27 OF 35 REGISTRY COPYRIGHT 2002 ACS  
RN 385384-45-2 REGISTRY  
CN Carbamic acid, [4-[(7R,8S,17S,18R)-7,8,17,18-tetrahydro-7,8,17,18-tetrahydroxy-15-(4-methoxyphenyl)-21H,23H-porphin-5-yl]phenyl]-,

**9H-fluoren-9-ylmethyl ester, rel- (9CI) (CA INDEX NAME)**

FS STEREOSEARCH  
 MF C48 H39 N5 O7  
 SR CA  
 LC STN Files: CA, CAPLUS, TOXCENTER

Relative stereochemistry.

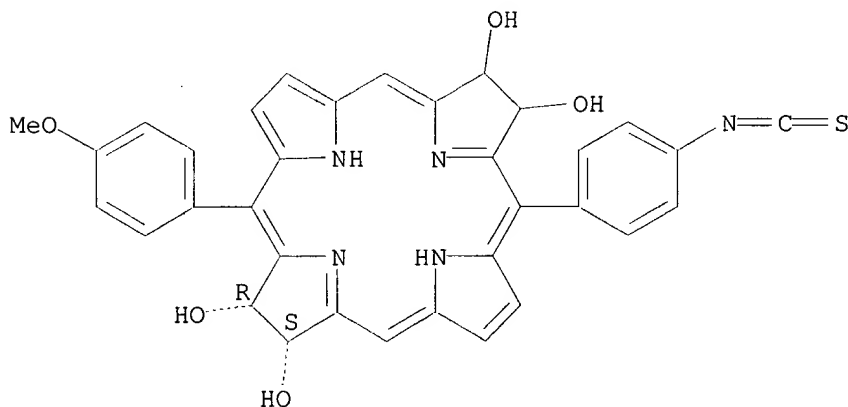


1 REFERENCES IN FILE CA (1962 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 136:69694

L49 ANSWER 28 OF 35 REGISTRY COPYRIGHT 2002 ACS  
 RN 318488-31-2 REGISTRY  
 CN **21H,23H-Porphine-7,8,17,18-tetrol, 7,8,17,18-tetrahydro-5-(4-isothiocyanatophenyl)-15-(4-methoxyphenyl)-, (17R,18S)-rel- (9CI)**  
 (CA INDEX NAME)  
 FS STEREOSEARCH  
 MF C34 H27 N5 O5 S  
 SR CA  
 LC STN Files: CA, CAPLUS

Relative stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

2 REFERENCES IN FILE CA (1962 TO DATE)

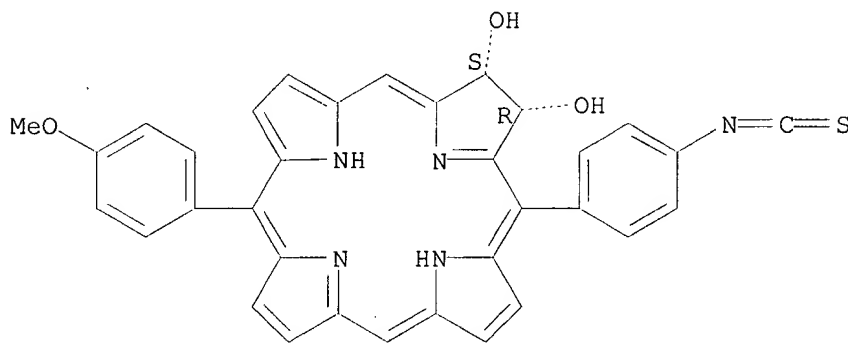
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2 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 136:321357

REFERENCE 2: 134:100684

L49 ANSWER 29 OF 35 REGISTRY COPYRIGHT 2002 ACS  
RN 318488-30-1 REGISTRY  
CN 21H,23H-Porphine-7,8-diol, 7,8-dihydro-5-(4-isothiocyanatophenyl)-15-(4-methoxyphenyl)-, (7R,8S)-rel- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C34 H25 N5 O3 S  
SR CA  
LC STN Files: CA, CAPLUS

Relative stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

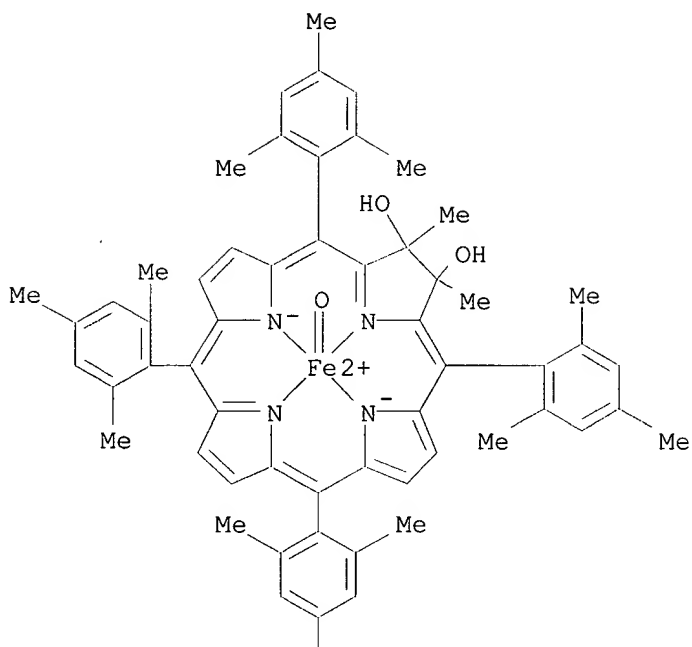
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1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 134:100684

L49 ANSWER 30 OF 35 REGISTRY COPYRIGHT 2002 ACS  
RN 167774-57-4 REGISTRY  
CN Iron, [rel-(7R,8R)-7,8-dihydro-7,8-dimethyl-5,10,15,20-tetrakis(2,4,6-trimethylphenyl)-21H,23H-porphine-7,8-diolato(2-)-.kappa.N21,.kappa.N22,.kappa.N23,.kappa.N24]oxo-, (SP-5-13)- (9CI) (CA INDEX NAME)  
MF C58 H58 Fe N4 O3  
CI CCS  
SR CA  
LC STN Files: CA, CAPLUS



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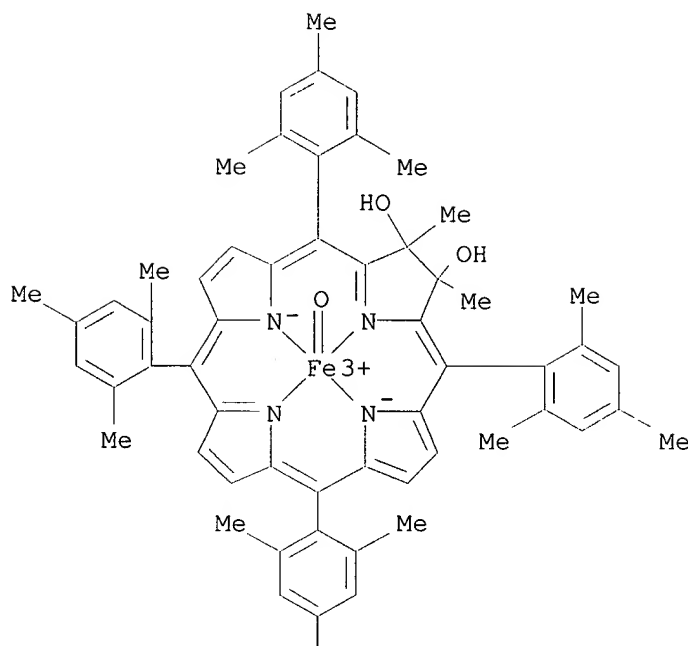


1 REFERENCES IN FILE CA (1962 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 123:216794

L49 ANSWER 31 OF 35 REGISTRY COPYRIGHT 2002 ACS  
 RN 167774-56-3 REGISTRY  
 CN Iron(1+), [rel-(7R,8R)-7,8-dihydro-7,8-dimethyl-5,10,15,20-tetrakis(2,4,6-trimethylphenyl)-21H,23H-porphine-7,8-diolato(2-)-.kappa.N21,.kappa.N22,.kappa.N23,.kappa.N24]oxo-, (SP-5-13)- (9CI) (CA INDEX NAME)  
 MF **C58 H58 Fe N4 O3**  
 CI CCS  
 SR CA  
 LC STN Files: CA, CAPLUS

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1 REFERENCES IN FILE CA (1962 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 123:216794

L49 ANSWER 32 OF 35 REGISTRY COPYRIGHT 2002 ACS

RN 167774-55-2 REGISTRY

CN Iron, [rel-(7R,8R)-7,8-dihydro-7,8-dimethyl-5,10,15,20-tetrakis(2,4,6-trimethylphenyl)-21H,23H-porphine-7,8-diolato(2-)-.kappa.N21,.kappa.N22,.kappa.N23,.kappa.N24](trifluoromethanesulfonato-O)-, (SP-5-13)- (9CI) (CA INDEX NAME)

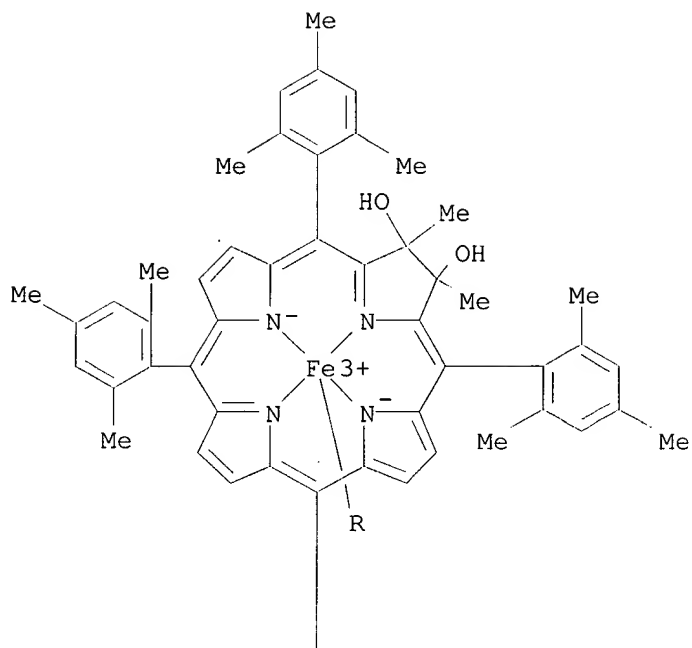
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CI CCS

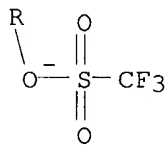
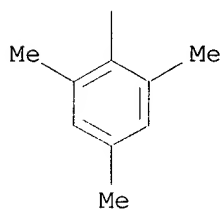
SR CA

LC STN Files: CA, CAPLUS

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1 REFERENCES IN FILE CA (1962 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 123:216794

L49 ANSWER 33 OF 35 REGISTRY COPYRIGHT 2002 ACS

RN 167774-54-1 REGISTRY

CN Iron, [rel-(7R,8R)-7,8-dihydro-7,8-dimethyl-5,10,15,20-tetrakis(2,4,6-trimethylphenyl)-21H,23H-porphine-7,8-diolato(2-)-.kappa.N21,.kappa.N22,.kappa.N23,.kappa.N24]hydroxy-, (SP-5-13)- (9CI)  
 (CA INDEX NAME)

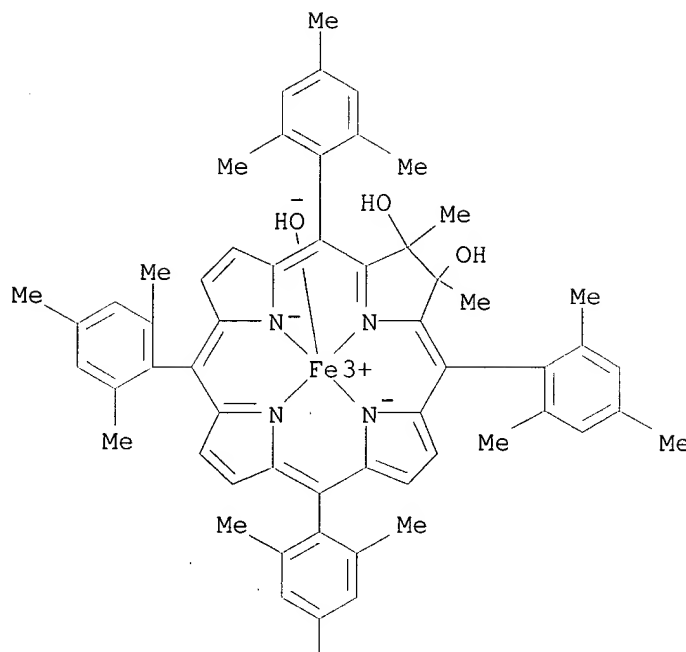
MF C58 H59 Fe N4 O3

CI CCS

SR CA

LC STN Files: CA, CAPLUS

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Me

1 REFERENCES IN FILE CA (1962 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 123:216794

L49 ANSWER 34 OF 35 REGISTRY COPYRIGHT 2002 ACS

RN 167774-53-0 REGISTRY

CN Iron(1+), chloro[rel-(7R,8R)-7,8-dihydro-7,8-dimethyl-5,10,15,20-tetrakis(2,4,6-trimethylphenyl)-21H,23H-porphine-7,8-diolato(2-)-.kappa.N21,.kappa.N22,.kappa.N23,.kappa.N24]-, (SP-5-13)-(9CI) (CA INDEX NAME)

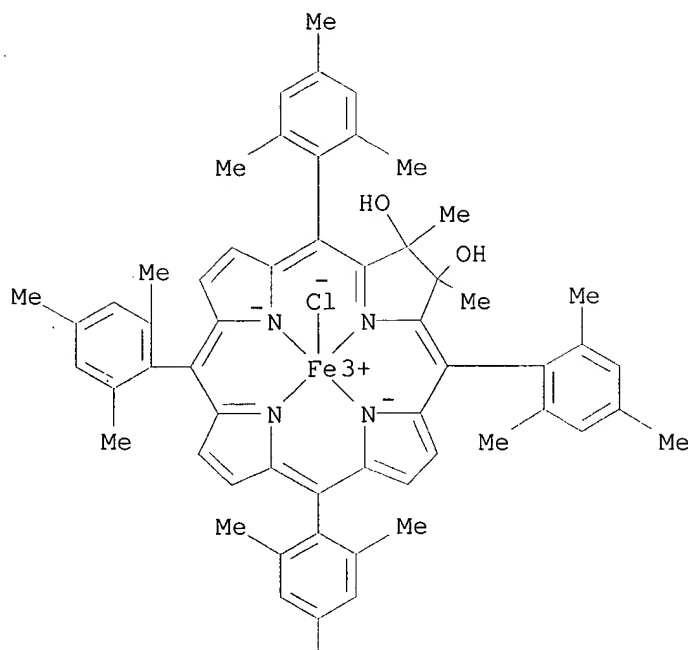
MF C58 H58 Cl Fe N4 O2

CI CCS

SR CA

LC STN Files: CA, CAPLUS

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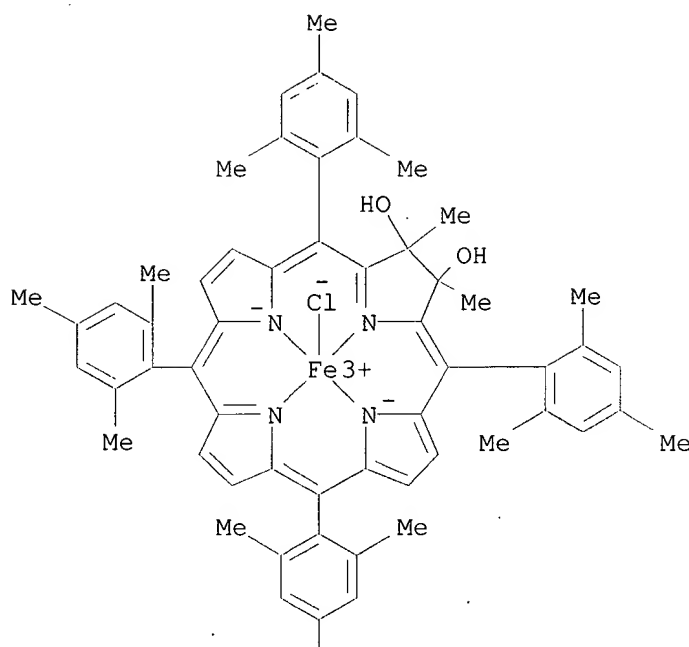


1 REFERENCES IN FILE CA (1962 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 123:216794

L49 ANSWER 35 OF 35 REGISTRY COPYRIGHT 2002 ACS  
 RN 167774-52-9 REGISTRY  
 CN Iron, chloro[rel-(7R,8R)-7,8-dihydro-7,8-dimethyl-5,10,15,20-tetrakis(2,4,6-trimethylphenyl)-21H,23H-porphine-7,8-diolato(2-)-.kappa.N21,.kappa.N22,.kappa.N23,.kappa.N24]-, (SP-5-13)- (9CI) (CA INDEX NAME)  
 MF C58 H58 Cl Fe N4 O2  
 CI CCS  
 SR CA  
 LC STN Files: CA, CAPLUS

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1 REFERENCES IN FILE CA (1962 TO DATE)  
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REFERENCE 1: 123:216794

=> d his 161-

(FILE 'REGISTRY' ENTERED AT 09:48:50 ON 03 NOV 2002)

FILE 'HCAPLUS' ENTERED AT 09:49:36 ON 03 NOV 2002

FILE 'REGISTRY' ENTERED AT 09:50:41 ON 03 NOV 2002

FILE 'HCAOLD' ENTERED AT 09:51:13 ON 03 NOV 2002

L61 0 S L49

FILE 'HCAPLUS' ENTERED AT 09:51:17 ON 03 NOV 2002

L62 4 S L49

L63 2 S L62 AND L1-L11

L64 4 S L62,L63

FILE 'USPATFULL, USPAT2' ENTERED AT 09:51:34 ON 03 NOV 2002

L65 0 S L49

=> fil hcaplus

FILE 'HCAPLUS' ENTERED AT 09:51:45 ON 03 NOV 2002

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FILE COVERS 1907 - 3 Nov 2002 VOL 137 ISS 19  
FILE LAST UPDATED: 1 Nov 2002 (20021101/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

CAS roles have been modified effective December 16, 2001. Please check your SDI profiles to see if they need to be revised. For information on CAS roles, enter HELP ROLES at an arrow prompt or use the CAS Roles thesaurus (/RL field) in this file.

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L64 ANSWER 1 OF 4 HCAPLUS COPYRIGHT 2002 ACS  
AN 2002:134544 HCAPLUS  
DN 136:321357  
TI Porphyrin, Chlorin, and Bacteriochlorin Isothiocyanates: Useful Reagents for the Synthesis of Photoactive Bioconjugates  
AU Sutton, J. M.; Clarke, O. J.; Fernandez, N.; Boyle, R. W.  
CS Department of Biological Sciences, University of Essex, Colchester, CO4 3SQ, UK  
SO Bioconjugate Chemistry (2002), 13(2), 249-263  
CODEN: BCCHES; ISSN: 1043-1802  
PB American Chemical Society  
DT Journal  
LA English  
CC 8-9 (Radiation Biochemistry)  
Section cross-reference(s): 9, 26  
AB A novel method for conjugating porphyrins and related mols. to proteins has been developed. The method, which involves synthesizing porphyrins, chlorins, and bacteriochlorins bearing a single amine-reactive isothiocyanate group represents a facile system for protein labeling with these photoactive species. Problems assocd. with the noncovalent binding of porphyrins to proteins are highlighted, and a method for purifying conjugates to yield exclusively covalently bound porphyrin protein species is demonstrated. Biol. activity of porphyrin-bovine serum albumin conjugates formed and purified by these methods is demonstrated using laser scanning confocal microscopy.  
ST porphyrin protein conjugate prepn carcinoma uptake  
IT Functional groups  
(isothiocyanato group; porphyrin-protein conjugate prepn. and tumor uptake)  
IT Carcinoma  
Conjugation (bond)  
Fluorescence  
Fluorescent indicators  
Human  
Microscopy

- (porphyrin-protein conjugate prepn. and tumor uptake)
- IT **Porphyrins**  
 RL: DGN (Diagnostic use); PKT (Pharmacokinetics); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (protein conjugates; porphyrin-protein conjugate prepn. and tumor uptake)
- IT Albumins, biological studies  
 RL: DGN (Diagnostic use); PKT (Pharmacokinetics); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (serum, porphyrin conjugates; porphyrin-protein conjugate prepn. and tumor uptake)
- IT **385384-58-7P 385384-59-8P 414866-60-7P 414866-61-8P**  
 RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)  
 (porphyrin-protein conjugate prepn. and tumor uptake)
- IT 2683-78-5DP, BacterioChlorin, derivs., protein conjugates 2683-84-3DP, Chlorin, derivs., protein conjugates  
 RL: DGN (Diagnostic use); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (porphyrin-protein conjugate prepn. and tumor uptake)
- IT 318488-18-5P 385384-43-0P  
 RL: PUR (Purification or recovery); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (porphyrin-protein conjugate prepn. and tumor uptake)
- IT 176446-62-1 214554-43-5 367277-50-7  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (porphyrin-protein conjugate prepn. and tumor uptake)
- IT 127800-97-9P 154960-65-3P 155165-82-5P 250764-51-3P 250764-53-5P  
 253666-30-7P 253666-33-0P 253666-35-2P 253666-41-0P 253666-46-5P  
**318488-31-2P** 385384-40-7P 385384-44-1P 385384-48-5P  
 385384-50-9P 385384-52-1P **385384-54-3P** 385384-75-8P  
 414866-48-1P 414866-49-2P 414866-50-5P 414866-51-6P 414866-52-7P  
 414866-53-8P 414866-54-9P 414866-55-0P 414866-56-1P 414866-57-2P  
**414866-58-3P 414866-59-4P**  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (porphyrin-protein conjugate prepn. and tumor uptake)
- RE.CNT 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD  
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L64 ANSWER 2 OF 4 HCAPLUS COPYRIGHT 2002 ACS

AN 2002:10481 HCAPLUS

DN 136:69694

TI Preparation of novel porphyrin and porphyrin-based chromophores which may be particularly useful in a range of photodynamic applications

IN Boyle, Ross William; Clarke, Oliver James; Sutton, Jonathan Mark; Greenman, John

PA Catalyst Biomedica Ltd., UK

SO PCT Int. Appl., 128 pp.

CODEN: PIXXD2

DT Patent

LA English

IC ICM C07D487-22

ICS C09K009-02; A61K031-40

CC 26-4 (Biomolecules and Their Synthetic Analogs)

Section cross-reference(s): 63, 74

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
	-----	----	-----	-----	-----
PI	WO 2002000662	A1	20020103	WO 2001-GB2846	20010626
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	AU 2001070748	A5	20020108	AU 2001-70748	20010626
PRAI	US 2000-214075P	P	20000626		
	GB 2001-13784	A	20010606		
	WO 2001-GB2846	W	20010626		
OS	MARPAT 136:69694				
GI					

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB The present invention relates to the prepn. of novel porphyrins of formula I [R1 = aryl moiety linked to a conjugating group which is capable of conjugating the chromophore to a polypeptide mol. for delivering said chromophore to a specific biol. target in vitro or in vivo; R2 = hydrophilic aryl; R3 = H, hydrophilic aryl, or hydrophilic non-arom. moiety] and related chlorin and bacteriochlorin chromophores and sets of porphyrin and porphyrin-based chromophores, which may be particularly useful in a range of photodynamic applications, including photochemotherapy and fluorescence anal. and imaging (no data). Thus, 4-acetamidobenzaldehyde and 3,5-dimethoxybenzaldehyde were stirred in

- propionic acid and treated with pyrrole to afford 5-(4-acetamidophenyl)-10,15,20-tris(3,5-dimethoxyphenyl)porphyrin (II) in 9.1%.
- ST porphyrin chlorin bacteriochlorin chromophore prepn photochemotherapy fluorescence analysis imaging
- IT Gel electrophoresis  
(SDS; elution of porphyrin-antibody bioconjugates from SDS PAGE utilizing micro-electroeluter)
- IT Cytometry  
(flow; prepn. of novel porphyrin and porphyrin-based chromophores which may be particularly useful in a range of photodynamic applications)
- IT AIDS (disease)  
Autoimmune disease  
Multiple sclerosis  
Rheumatoid arthritis  
(method for treating a disease or disorder which is characterized by the presence in the body of diseased or undesired cells, such as)
- IT Cytotoxicity  
(photo-; prepn. of novel porphyrin and porphyrin-based chromophores which may be particularly useful in a range of photodynamic applications)
- IT Confocal laser scanning microscopy  
Photodynamic therapy  
(prepn. of novel porphyrin and porphyrin-based chromophores which may be particularly useful in a range of photodynamic applications)
- IT Suzuki coupling reaction  
(prepn. of novel porphyrin and porphyrin-based chromophores which may be particularly useful in a range of photodynamic applications via)
- IT 253666-30-7P 253666-33-0P 268737-71-9P 318488-18-5P 385384-43-0P  
385384-44-1P **385384-45-2P 385384-46-3P** 385384-48-5P  
385384-49-6P 385384-50-9P 385384-51-0P  
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)  
(prepn. of novel porphyrin and porphyrin-based chromophores which may be particularly useful in a range of photodynamic applications)
- IT 253666-35-2P 318488-06-1P 385384-47-4P 385384-52-1P 385384-53-2P  
**385384-54-3P 385384-55-4P 385384-56-5P**  
**385384-57-6P 385384-58-7P 385384-59-8P**  
385384-60-1P 385384-61-2P 385384-62-3P 385384-63-4P  
**385384-64-5P 385384-65-6P** 385384-66-7P  
385384-67-8P 385384-68-9P 385384-69-0P  
385384-70-3P 385384-71-4P 385384-72-5P  
**385384-73-6P 385384-74-7P** 385384-75-8P  
**385384-76-9P 385384-77-0P 385384-79-2P**  
**385384-83-8P 385384-84-9P 385384-85-0P**  
**385384-86-1P** 385384-87-2P  
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(prepn. of novel porphyrin and porphyrin-based chromophores which may be particularly useful in a range of photodynamic applications)
- IT 86-81-7, 3,4,5-Trimethoxybenzaldehyde 109-97-7, Pyrrole 122-85-0,  
4-Acetamidobenzaldehyde 123-11-5, reactions 500-22-1,  
3-Pyridinecarboxaldehyde 872-85-5, 4-Pyridinecarboxaldehyde 7311-34-4,  
3,5-Dimethoxybenzaldehyde 28920-43-6, 9-Fluorenylmethyl chloroformate  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(prepn. of novel porphyrin and porphyrin-based chromophores which may be particularly useful in a range of photodynamic applications)
- IT 127800-97-9P 154960-65-3P 167482-90-8P 176446-62-1P 214554-43-5P  
250764-51-3P 250764-53-5P 385384-40-7P 385384-41-8P 385384-42-9P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(prepn. of novel porphyrin and porphyrin-based chromophores which may

be particularly useful in a range of photodynamic applications)

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L64 ANSWER 3 OF 4 HCAPLUS COPYRIGHT 2002 ACS

AN 2000:831421 HCAPLUS

DN 134:100684

TI Functionalized diphenylchlorins and bacteriochlorins: their synthesis and bioconjugation for targeted photodynamic therapy and tumor cell imaging

AU Sutton, Jonathan M.; Fernandez, Nelson; Boyle, Ross W.

CS Department of Biological Sciences, University of Essex, Colchester, CO4 3SQ, UK

SO Journal of Porphyrins and Phthalocyanines (2000), 4(7), 655-658

CODEN: JPPHFZ; ISSN: 1088-4246

PB John Wiley & Sons Ltd.

DT Journal

LA English

CC 26-7 (Biomolecules and Their Synthetic Analogs)

Section cross-reference(s): 9, 22

OS CASREACT 134:100684

AB A range of 5,15-diphenylporphyrins with sym. and unsym. substitution patterns were subjected to osmium tetroxide-mediated dihydroxylations. The resulting chlorins and bacteriochlorins present an important group of compds. for studying structure-activity relationships of photodynamic sensitizers. The regioselectivity of the dihydroxylation of various

5,15-diphenylporphyrins with unsym. substitution patterns was also examd. Both diphenylchlorin diol (DPC) and diphenylbacteriochlorin tetrol (DPBC) examples were converted into reactive isothiocyanates and conjugated with bovine serum albumin (BSA).

ST porphyrin diphenyl dihydroxylation regioselective; chlorin diphenyl dihydroxy tetrahydroxy prepn; diphenylchlorin bacteriochlorin isothiocyanate conjugate BSA

IT **Porphyrins**

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (chlorins, di-Ph; synthesis and bioconjugation of functionalized diphenylchlorins and bacteriochlorins for targeted photodynamic therapy and tumor cell imaging)

IT Albumins, biological studies

RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process) (conjugates; synthesis and bioconjugation of functionalized diphenylchlorins and bacteriochlorins for targeted photodynamic therapy and tumor cell imaging)

IT Dihydroxylation

(stereoselective; synthesis and bioconjugation of functionalized diphenylchlorins and bacteriochlorins for targeted photodynamic therapy and tumor cell imaging)

IT Fluorescence

UV and visible spectra (synthesis and bioconjugation of functionalized diphenylchlorins and bacteriochlorins for targeted photodynamic therapy and tumor cell imaging)

IT 318488-18-5P 318488-24-3P

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (synthesis and bioconjugation of functionalized diphenylchlorins and bacteriochlorins for targeted photodynamic therapy and tumor cell imaging)

IT 318488-06-1P 318488-12-9P 318488-23-2P 318488-29-8P

**318488-30-1DP**, conjugate with BSA **318488-31-2DP**, conjugate with BSA  
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (synthesis and bioconjugation of functionalized diphenylchlorins and bacteriochlorins for targeted photodynamic therapy and tumor cell imaging)

IT 22112-89-6, 5,15-Diphenylporphyrin 128374-05-0 253666-33-0  
268737-71-9 318488-01-6 318488-02-7 318488-13-0 318488-14-1  
318488-15-2 318488-16-3 318488-17-4

RL: RCT (Reactant); RACT (Reactant or reagent) (synthesis and bioconjugation of functionalized diphenylchlorins and bacteriochlorins for targeted photodynamic therapy and tumor cell imaging)

IT 165336-21-0P 318488-03-8P 318488-04-9P 318488-05-0P 318488-07-2P  
318488-08-3P 318488-10-7P 318488-11-8P 318488-19-6P 318488-20-9P  
318488-21-0P 318488-22-1P 318488-25-4P 318488-26-5P 318488-27-6P  
318488-28-7P

RL: SPN (Synthetic preparation); PREP (Preparation) (synthesis and bioconjugation of functionalized diphenylchlorins and bacteriochlorins for targeted photodynamic therapy and tumor cell imaging)

RE.CNT 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD

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L64 ANSWER 4 OF 4 HCAPLUS COPYRIGHT 2002 ACS

AN 1995:751119 HCAPLUS

DN 123:216794

TI Compound I and II Analogs of a Chlorin

AU Jayaraj, K.; Gold, A.; Austin, R. N.; Mandon, D.; Weiss, R.; Turner, J.; Bill, E.; Muether, M.; Trautwein, A. X.

CS Department of Environmental Sciences and Engineering, University of North Carolina, Chapel Hill, NC, 27599, USA

SO Journal of the American Chemical Society (1995), 117(35), 9079-80

CODEN: JACSAT; ISSN: 0002-7863

PB American Chemical Society

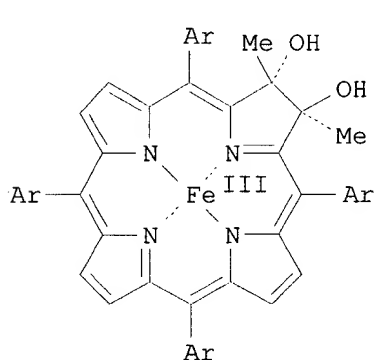
DT Journal

LA English

CC 78-7 (Inorganic Chemicals and Reactions)

Section cross-reference(s): 7, 26, 72

GI



AB I (Ar = 2,4,6-trimethylphenyl) with coordinated chloride, hydroxide and triflate, were prepd. The 1st electrochem. oxidn. of both the ligand (LH2) and I(Cl) are reversible and are ligand-centered. Oxidn. of I(OH) by m-chloroperbenzoic acid gave [FeIVOL]<sup>+</sup>, a model of the compd. I analog of chlorin, transients of catalases and [FeIVOL], a model of the compd. II analog of chlorin. [FeIVOL]<sup>+</sup> decays to [FeIVOL]. The complexes were characterized by various techniques such as EPR, Moessbauer, UV-visible and resonance Raman spectroscopy.

ST chlorin compd I II analog; catalase transient model iron 4 complex; ferryl chlorin pi cation radical; electrochem chlorin iron complex

IT Enzyme functional sites

RL: BSU (Biological study, unclassified); BIOL (Biological study)  
(ferryl chlorin complexes as models of compd. I and II analogs of catalase)

IT Oxidation, electrochemical  
(of chlorin deriv. and metal-free base)

IT 167774-53-0 167936-43-8  
 RL: FMU (Formation, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); FORM (Formation, nonpreparative); PROC (Process); RACT (Reactant or reagent) (electrochem. formation and elec. potential of couple contg.)

IT 9001-05-2, Catalase  
 RL: BSU (Biological study, unclassified); BIOL (Biological study) (ferryl chlorin complexes as models of compd. I and II analogs of)

IT 167774-52-9P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (prepn. and metatheses)

IT 167774-54-1P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (prepn. and oxidn.)

IT 167774-51-8P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (prepn. and reaction with ferrous chloride)

IT 167774-56-3P  
 RL: BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent) (prepn. as compd. I analog of chlorin and decay to compd. II analog)

IT 167774-57-4P  
 RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation) (prepn. as compd. II analog of chlorin)

IT 167774-55-2P  
 RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of)

IT 167774-58-5, 2,3-Dioxo-meso-tetramesitylporphyrin  
 RL: RCT (Reactant); RACT (Reactant or reagent) (reaction with methyllithium)

=> d his

(FILE 'HOME' ENTERED AT 09:05:55 ON 03 NOV 2002)  
 SET COST OFF

FILE 'HCAPLUS' ENTERED AT 09:06:33 ON 03 NOV 2002

E DOLPHIN D/AU

L1	484	S E3-E6
		E BRUCKNER C/AU
L2	53	S E3,E4,E11
		E MACALPINE J/AU
L3	12	S E5-E10
		E MAC ALPINE J/AU
L4	532	S L1-L3
L5	37	S L4 AND (?CHLORIN OR ?CHLORINS)
		E PORPHYRIN/CT
		E E7+ALL
L6	73912	S E4+NT
L7	189	S L4 AND L6
L8	305	S ?PORPHYR? AND L4
L9	321	S L5,L7,L8
L10	1	S L1 AND L2 AND L3
L11	531	S L4,L9 NOT L10
		SEL RN L10

FILE 'REGISTRY' ENTERED AT 09:10:06 ON 03 NOV 2002

L12 43 S E1-E43  
L13 30 S L12 AND NR>=7  
L14 STR  
L15 50 S L14  
L16 SCR 1868  
L17 STR L14  
L18 50 S L17 AND L16  
L19 50 S L17  
L20 71959 S L17 FUL  
L21 40100 S L20 AND 46.150.18/RID  
L22 36698 S L14 FUL SUB=L21  
SAV TEMP L22 FAY551/A  
L23 STR L17  
L24 5 S L23 SAM SUB=L22  
L25 102 S L23 FUL SUB=L22  
SAV L25 FAY551A/A  
L26 62 S L25 AND O>=4  
L27 STR L23  
L28 30 S L27 FUL SUB=L25  
SAV L28 FAY551B/A  
L29 4 S L28 AND (C44H34N4O4 OR C33H25N5O4S OR C32H26N4O4)  
L30 26 S L28 NOT L29  
L31 25 S L30 NOT C36H30N4O8  
L32 1 S L30 NOT L31  
L33 STR L23  
L34 STR L33  
L35 2 S L34 SAM SUB=L25  
L36 75 S L34 FUL SUB=L25  
SAV L36 FAY551C/A  
L37 49 S L36 NOT L28  
L38 1 S L37 AND C60H64N4O2  
L39 2 S L37 AND (C36H28N4O6 OR C52H40N4O10)  
L40 46 S L37 NOT L38,L39  
L41 71 S L31,L40  
L42 12 S L12 AND L41  
L43 1 S L12 AND L32,L38  
L44 2 S L32,L38,L43  
L45 30 S L12 AND L20  
L46 17 S L45 NOT L41-L44  
L47 3 S L25 AND IDS/CI  
L48 74 S L41,L47  
L49 35 S L48 AND (ACETAMIDE OR ISOTHIOCYAN? OR CARBAMIC OR FE/ELS)  
L50 39 S L48 NOT L49  
SAV L48 FAY551D/A  
SAV L50 FAY551E/A

FILE 'HCAOLD' ENTERED AT 09:47:14 ON 03 NOV 2002

L51 0 S L50

FILE 'HCAPLUS' ENTERED AT 09:47:18 ON 03 NOV 2002

L52 8 S L50  
L53 3 S L51 AND L1-L11  
L54 7 S L52,L53 AND (PY<=2000 OR PRY<=2000 OR AY<=2000)  
L55 2 S L44  
L56 2 S L55 AND L1-L11  
L57 8 S L52-L54  
L58 2 S L55,L56

FILE 'USPATFULL, USPAT2' ENTERED AT 09:48:31 ON 03 NOV 2002

L59 0 S L50  
L60 0 S L44

FILE 'REGISTRY' ENTERED AT 09:48:50 ON 03 NOV 2002

FILE 'HCAPLUS' ENTERED AT 09:49:36 ON 03 NOV 2002

FILE 'REGISTRY' ENTERED AT 09:50:41 ON 03 NOV 2002

FILE 'HCAOLD' ENTERED AT 09:51:13 ON 03 NOV 2002

L61 0 S L49

FILE 'HCAPLUS' ENTERED AT 09:51:17 ON 03 NOV 2002

L62 4 S L49

L63 2 S L62 AND L1-L11

L64 4 S L62,L63

FILE 'USPATFULL, USPAT2' ENTERED AT 09:51:34 ON 03 NOV 2002

L65 0 S L49

FILE 'HCAPLUS' ENTERED AT 09:51:45 ON 03 NOV 2002